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SciDAC-2: National Computational Infrastructure for Lattice Gauge Theory
University of Utah Component
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1 Brief Description of Accomplishments

The overall structure and accomplishments of this project are described in the SciDAC-2 project-wide final report. This report identifies the part done by the three MILC collaboration institutions, the University of Arizona, Indiana University, and the University of Utah.

The MILC collaboration consists of approximately ten senior and eight junior members at ten institutions, mostly in the USA.¹ Almost all of its scientific work is done with the MILC code, an integrated package of some 200,000 lines of scientific application codes and a library of generic supporting codes. It has been in use worldwide and freely available to the public since the early 1990's, and has grown and evolved over the years to meet our evolving physics goals and rapid changes in computer architecture and capability.

Under SciDAC-2, three MILC-collaboration institutions, the University of Arizona, Indiana University, and the University of Utah, were responsible for a large number of important revisions to the code that exploit the evolving

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SciDAC code suite. These institutions have also contributed important new SciDAC modules. These changes have made the MILC code much more flexible, they have allowed us to keep abreast of our changing scientific objectives. As a consequence, they have enabled rapid scientific progress.

Over the six years of the SciDAC-2 grant, the three MILC institutions received support for one (approximately) 0.5 FTE postdoctoral research associate each. We list accomplishments and publications resulting from this support:

1.1 Arizona

Work at the University of Arizona was done by postdoctoral researchers Dru Renner (–Sep. 2007), currently at Jefferson Lab, Alexei Bazavov (Sep. 2007–Aug. 2010), currently at Brookhaven National Laboratory and Jongjeong Kim (Nov. 2010–present), under the supervision of the PI, Doug Toussaint.

Operation of the QCDOC During the first part of the proposal period the University of Arizona was responsible for the implementation and operation of the MILC code on the QCDOC, the special purpose machine at Brookhaven National Laboratory (BNL). This included testing the codes and making the necessary modifications to get them to run on the QCDOC, and developing and maintaining the scripts needed at the top level to use the QCD codes in projects. This also required arranging for the movement of lattices and output files to and from BNL. The QCDOC was used successfully in generating many of the lattice ensembles made with the Asqtad fermion action, and these ensembles were later used by many lattice projects in both high energy and nuclear physics [1].

Implementation of the highly improved staggered quark (HISQ) algorithm Following the retirement of the QCDOC, the postdocs at the University of Arizona concentrated on the development of the “Highly Improved Staggered Quark” (HISQ) action introduced by the HPQCD collaboration. Specifically, they completed the programming of the code for the “fermion force”, which is necessary to generate ensembles with dynamical HISQ quarks, and for the projection of intermediate matrices onto unitary matrices. These routines were integrated into the MILC code suite, making possible the generation of large lattice ensembles using this action.

This algorithm has become a mainstay of our current physics efforts. It is yielding greatly improved control of discretization errors, which, in turn, is producing higher precision results [2, 3, 4, 5, 6].

Porting the HISQ algorithm into SciDAC Level 3 Optimized QOP (Level 3) versions of the HISQ routines were developed, and these have now been placed in the production environments for this project. This step is essential for taking advantage of architecture-specific optimizations in the SciDAC code suite [7].

Production of gauge field configurations with HISQ These gauge configurations are the basis for many physics analyses, including spectroscopy, decay constants, and a wide variety of weak matrix elements [1]. We publish worldwide the gauge field configurations we produce [8].

1.2 Indiana University

Work at Indiana University was done by postdoctoral researchers Subhasish Basak (Jan. 2007–Sep. 2008), at the National Institute of Science Education and Research, Bhubaneswar, India, and Aaron Torok (Sep. 2009–June 2011), currently at FEI Corporation, under the supervision of the PI, Steven Gottlieb.

Single-GPU code for asqtad lattice generation This work, done in collaboration with Guochun Shi of the National Center for Supercomputing Applications (NCSA) developed all the major components for asqtad lattice generation. The code was incorporated into the SciDAC QUDA library. [9, 10]. This is a milestone on the path to multi-GPU capability.

Multi-GPU gauge-force and fat-Naik solver This work, again with G. Shi, developed and benchmarked an improved gauge-force routine and a fat-Naik solver for multi-GPU operation [11, 12].

Integration of the MILC code with the SciDAC QUDA multi-GPU fat-Naik solver This capability gives our code a factor of four or more speedup for some of our analysis projects [11, 12, 13]. The code has been put into production measuring electromagnetic splittings of hadron masses [14].

Development of code for heavy baryon spectroscopy This new MILC code module made it possible to do the spectroscopy of baryons containing a charm or bottom quark [15, 16].

1.3 University of Utah

Work at the University of Utah was done by postdoctoral researchers Tommy Burch (Oct. 2007–Sep. 2008), currently at the University of Regensburg, Germany, Bugra Oktay (Sep. 2008–Feb. 2011), currently at the Utah Center for Advanced Imaging Research, Ludmila Levkova (Aug. 2012–Sep. 2012), and Justin Foley (Oct. 2010–Jul. 2012) under the supervision of the PI, Carleton DeTar.

Two major releases of the MILC code suite These revisions provide support for the HISQ algorithm, greatly expanded support for hadron interpolating source operators, the FFTW (Fourier transform) package, the PRIMME (eigenvalue) package, random color-wall sources, momentum twists, open-meson code for B Bbar mixing calculation, HISQ equation of state, etc. [17]. The new

features of the code are yielding new physics results [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37].

A user manual for the MILC code suite This 70-page user manual, developed and provided with the code release, describes how to build and operate the code [17].

Development of QUDA GPU HISQ link-fattening and fermion force modules These are the first steps toward developing the ability to do full HISQ hybrid molecular dynamics calculations on multiple GPU's.

Testing the improved heavy-quark Oktay-Kronfeld action This action is designed to do for heavy quarks what the asqtad and HISQ actions do for light quarks, namely reducing considerably the lattice discretization errors. Work is still under way [38].

2 Publications with multiagency support resulting from this work

The publications listed below resulted from collaborative work with significant involvement of the three SciDAC institutions in the MILC collaboration, namely the University of Arizona, Indiana University, and the University of Utah. Since this is a multi-institutional collaboration, other agency support (NSF) and other DOE awards provided partial support for collaboration members. Those awards support research with a wide range of DOE and NSF physics goals. The DOE award described in this final report was specifically intended to support the development of community software for achieving efficiently the physics goals of the other awards. In the previous section we have outlined the contributions of the three SciDAC institutions in the collaboration. The publications and URL documents listed below describe the developed software itself and report results of physics research in which the software product was an essential component.

References

- [1] A. Bazavov, C. Bernard, C. DeTar, S. Gottlieb, U.M. Heller, J.E. Hetrick, J. Laiho, L. Levkova, P.B. Mackenzie, M.B. Oktay, R. Sugar, D. Toussaint, and R.S. Van de Water. Nonperturbative QCD simulations with 2+1 flavors of improved staggered quarks. *Reviews of Modern Physics*, 82:1349–1417, 2010.
- [2] A. Bazavov et al. HISQ action in dynamical simulations. *PoS, LATTICE2008:033*, 2008, [arXiv:0903.0874].
- [3] A. Bazavov et al. Progress on four flavor QCD with the HISQ action. *PoS, LAT2009:123*, 2009, [arXiv:0911.0869].

- [4] A. Bazavov, C. Bernard, C. DeTar, W. Freeman, Steven Gottlieb, et al. Simulations with dynamical HISQ quarks. *PoS*, LATTICE2010:320, 2010, [arXiv:1012.1265].
- [5] A. Bazavov et al. Scaling studies of QCD with the dynamical HISQ action. *Phys.Rev.*, D82:074501, 2010, [arXiv:1004.0342].
- [6] A. Bazavov et al. Properties of light pseudoscalars from lattice QCD with HISQ ensembles. *PoS*, LATTICE2011:107, 2011, [arXiv:1111.4314].
- [7] USQCD Collaboration. Usqcd software: <http://usqcd.jlab.org/>.
- [8] Carleton E. DeTar. Sharing lattices throughout the world: An ILDG status report. *PoS*, LAT2007:009, 2007, [arXiv:0710.1660].
- [9] Steven Gottlieb, Guochun Shi, Aaron Torok, and Volodymyr Kindratenko. QUDA programming for staggered quarks. *PoS*, LATTICE2010:026, 2010.
- [10] G. Shi, S. Gottlieb, A. Torok, and V. Kindratenko. Accelerating Quantum Chromodynamics Calculations with GPUs. In *Proc. Symposium on Application Accelerators in HPC (SAAHPC10)*, Knoxville, TN, July 2010.
- [11] G. Shi, S. Gottlieb, A. Torok, and V. Kindratenko. Design of MILC lattice QCD application for GPU clusters. In *Proceedings of the 2011 IEEE Parallel and Distributed Processing Symposium*, IPDPS '11. IEEE, 2011.
- [12] R. Babich and M. A. Clark and B. Joó and G. Shi and R. C. Brower and S. Gottlieb. Scaling Lattice QCD beyond 100 GPUs. In *Proceedings of the 2011 ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '11. IEEE Computer Society, 2011.
- [13] R. Babich and R. C. Brower and M. A. Clark and S. Gottlieb and B. Joó and G. Shi. Progress on the QUDA code suite. *PoS*, LATTICE2011:033, 2011.
- [14] A. Torok, S. Basak, A. Bazavov, C. Bernard, C. DeTar, et al. Electromagnetic splitting of charged and neutral mesons. *PoS*, LATTICE2010:127, 2010.
- [15] Heechang Na and Steven Gottlieb. Heavy baryon mass spectrum from lattice QCD with 2+1 dynamical sea quark flavors. *PoS*, LATTICE2008:119, 2008, [arXiv:0812.1235].
- [16] Heechang Na and Steven Gottlieb. Charm and bottom heavy baryon mass spectrum from lattice QCD with 2+1 flavors. *PoS*, LAT2007:124, 2007, [arXiv:0710.1422].
- [17] MILC Collaboration. MILC Code: http://www.physics.utah.edu/~detar/milc/milc_qcd.html.

- [18] Richard Todd Evans, Elvira Gamiz, Aida El-Khadra, and Andreas Kronfeld. B-Bbar Mixing and Matching with Fermilab Heavy Quarks. *PoS, LAT2009:245*, 2009, [arXiv:0911.5432].
- [19] C. Bouchard, A.X. El-Khadra, E.D. Freeland, E. Gamiz, and A.S. Kronfeld. B_s^0 and B^0 Mixing in the Standard Model and Beyond: A Progress Report. *PoS, LATTICE2010:299*, 2010, [arXiv:1011.2570].
- [20] Jon A. Bailey et al. $B \rightarrow D^* \ell \nu$ at zero recoil: an update. *PoS, LATTICE2010:311*, 2010, [arXiv:1011.2166].
- [21] Jon A. Bailey, A. Bazavov, C. Bernard, C.M. Bouchard, C. DeTar, et al. $B_s \rightarrow D_s/B \rightarrow D$ Semileptonic Form-Factor Ratios and Their Application to $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-)$. 2012, [arXiv:1202.6346].
- [22] C. Bernard et al. B Mixing in the Standard Model and Beyond: Lattice QCD. 2011, [arXiv:1111.2968].
- [23] C.M. Bouchard, E.D. Freeland, C. Bernard, A.X. El-Khadra, E. Gamiz, et al. Neutral B mixing from 2+1 flavor lattice-QCD: the Standard Model and beyond. *PoS, LATTICE2011:274*, 2011, [arXiv:1112.5642].
- [24] Si-Wei Qiu et al. Semileptonic B to D Decays at Nonzero Recoil with 2+1 Flavors of Improved Staggered Quarks. *PoS, LATTICE2011*, 2011, [arXiv:1111.0677].
- [25] Daping Du, Carleton DeTar, Andreas Kronfeld, Jack Laiho, Yannick Meurice, et al. Semileptonic Form Factor ratio $B_s \rightarrow D_s/B \rightarrow D$ and Its Application to $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-)$. 2011, [arXiv:1111.1796].
- [26] E. Gamiz, C. DeTar, A.X. El-Khadra, A.S. Kronfeld, P.B. Mackenzie, et al. Calculation of $K \rightarrow \pi \ell \nu$ Form Factors with $N_f = 2+1$ Flavors of Staggered Quarks. 2011, [arXiv:1111.2021].
- [27] E.T. Neil et al. B and D meson decay constants from 2+1 flavor improved staggered simulations. *PoS, LATTICE2011:320*, 2011, [arXiv:1112.3978].
- [28] A. Bazavov et al. B- and D-meson decay constants from three-flavor lattice QCD. *Phys.Rev.*, D85:114506, 2012, [arXiv:1112.3051].
- [29] A. Bazavov et al. Two-point Correlator Fits on HISQ Ensembles. 2012, [arXiv:1212.0613].
- [30] Carleton DeTar, A.S. Kronfeld, Song-Haeng Lee, L. Levkova, D. Mohler, et al. Charmonium mass splittings at the physical point. 2012, [arXiv:1211.2253].
- [31] Si-Wei Qiu, Carleton DeTar, Daping Du, Andreas S. Kronfeld, Jack Laiho, et al. Semileptonic B to D decays at nonzero recoil with 2+1 flavors of improved staggered quarks. An update. 2012, [arXiv:1211.2247].

- [32] E. Gamiz, J.A. Bailey, A. Bazavov, C. Bernard, C. Bouchard, et al. Kaon semileptonic decay form factors with HISQ valence quarks. 2012, [arXiv:1211.0751].
- [33] A. Bazavov et al. Pseudoscalar meson physics with four dynamical quarks. 2012, [arXiv:1210.8431].
- [34] S. Basak et al. Status of the MILC calculation of electromagnetic contributions to pseudoscalar masses. 2012, [arXiv:1210.8157].
- [35] Jon A. Bailey, A. Bazavov, C. Bernard, C.M. Bouchard, C. DeTar, et al. Refining new-physics searches in $B^- \rightarrow D\tau\nu$ decay with lattice QCD. *Phys.Rev.Lett.*, 109:071802, 2012, [arXiv:1206.4992].
- [36] A. Bazavov, C. Bernard, C.M. Bouchard, C. DeTar, M. Di Pierro, et al. Neutral B-meson mixing from three-flavor lattice QCD: Determination of the SU(3)-breaking ratio ξ . *Phys.Rev.*, D86:034503, 2012, [arXiv:1205.7013].
- [37] A. Bazavov et al. Fluctuations and Correlations of net baryon number, electric charge, and strangeness: A comparison of lattice QCD results with the hadron resonance gas model. *Phys.Rev.*, D86:034509, 2012, [arXiv:1203.0784].
- [38] C. DeTar, A.S. Kronfeld, and M.B. Oktay. Numerical Tests of the Improved Fermilab Action. *PoS*, LATTICE2010:234, 2010, [arXiv:1011.5189].

3 University of Utah Personnel

The award provided only approximately 0.5 FTE support for these personnel with occasional interruptions. The NSF provided the balance of the salary in support of physics research.

Name	Dates	Current location
Tommy Burch	Oct. 2007–Sep. 2008	University of Regensburg, Germany
Bugra Oktay	Sep. 2008–Feb. 2011	Utah Center for Advanced Imaging Research
Justin Foley	Oct. 2010–Jul. 2012	Continuing at Univ. Utah
Ludmila Levkova	Aug. 2012–Sep. 2012	Continuing at Univ. Utah

4 Unexpended Funds

All funds were expended.

Scaling studies of QCD with the dynamical highly improved staggered quark action

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We study the lattice spacing dependence, or scaling, of physical quantities using the highly improved staggered quark (HISQ) action introduced by the HPQCD/UKQCD Collaboration, comparing our results to similar simulations with the asqtad fermion action. Results are based on calculations with lattice spacings approximately 0.15, 0.12, and 0.09 fm, using four flavors of dynamical HISQ quarks. The strange and charm quark masses are near their physical values, and the light-quark mass is set to 0.2 times the strange-quark mass. We look at the lattice spacing dependence of hadron masses, pseudoscalar meson decay constants, and the topological susceptibility. In addition to the commonly used determination of the lattice spacing through the static quark potential, we examine a determination proposed by the HPQCD Collaboration that uses the decay constant of a fictitious “unmixed $s\bar{s}$ ” pseudoscalar meson. We find that the lattice artifacts in the HISQ simulations are much smaller than those in the asqtad simulations at the same lattice spacings and quark masses.

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I. INTRODUCTION AND MOTIVATION

The “highly improved staggered quark,” or HISQ, action was developed by the HPQCD/UKQCD Collaboration to reduce the lattice artifacts associated with staggered quarks in lattice QCD calculations [1–3]. While significantly more expensive than the asqtad action used in the MILC Collaboration’s long-running program of QCD simulations with three dynamical quark flavors [4], it is still very economical compared with nonstaggered quark actions.

The initial studies of the HISQ action by the HPQCD/UKQCD Collaboration demonstrated the reduction of taste symmetry breaking and improvements in the dispersion relation for the charm quark by using the HISQ action for valence quarks on quenched lattices and lattices generated with asqtad sea quarks [1–3]. Further work with this action, again implemented for the valence quarks with asqtad sea quarks, has demonstrated impressive precision for charmonium and heavy-light meson physics [5–7].

As a first stage in a complete program of QCD simulations using the HISQ action for dynamical quarks, we have generated ensembles of lattices at three different lattice spacings with four flavors of dynamical quarks, where the light-quark mass is fixed at two-tenths of the strange-quark mass, and the strange and charm quark masses are near their physical values. This allows us to test scaling, or dependence of calculated quantities on the lattice spacing. The purpose of this paper is to report on these tests at fixed quark mass. Where possible, we compare the lattice spacing dependence of physical quantities with the HISQ action to their dependence using the asqtad action at the same quark mass and lattice spacings. We look at the static quark potential, splittings among the different tastes of pions, masses of the rho and nucleon, pseudoscalar meson decay constants, and the topological susceptibility. We emphasize that all of this is done at a fixed, and unphysically large, light-quark mass—our purpose here is to make a controlled study of the dependence on lattice spacing.

II. METHODS AND LATTICE DATA

There are four major differences between these HISQ simulations and our earlier asqtad simulations.

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TABLE I. Parameters of the HISQ runs with $m_l = 0.2m_s$. Here ϵ_N is the correction for the three-link (Naik) term in the charm quark action. These values differ slightly from the expression in Appendix A because they do not include the distinction between bare and tree-level quark mass [see Eq. (24) in Ref. [3]]. The expression in Appendix A is used in all more recent ensembles. The number of equilibrated lattices is N_{lats} . The separation of the lattices in simulation time is S_t , the length of a trajectory in simulation time is L_t , the molecular dynamics step size is ϵ , and the fraction of trajectories accepted is “Acc.” Our definition of the step size is such that there is one evaluation of the fermion force per step, so a complete cycle of the Omelyan integration algorithm includes two fermion-action steps and six gauge-action steps. The physical lattice spacing given in this table uses the three flavor determination of $r_1 = 0.3117(6)_{(-31)}^{(+12)}$ fm made using f_π to set the scale on the asqtad ensembles [9]. It should be noted that when chiral and continuum limits of $2 + 1 + 1$ flavor calculations are completed, a $2 + 1 + 1$ flavor determination of r_1 will supercede this.

$\frac{10}{g^2}$	am_l	am_s	am_c	ϵ_N	Size	u_0	N_{lats}	S_t	L_t	ϵ	Acc.	r_1/a	a (fm)
5.8	0.013	0.065	0.838	-0.3582	$16^3 \times 48$	0.855 35	1021	5	1.0	0.033	0.73	2.041(10)	$0.1527_{(-16)}^{(+7)}$
6.0	0.0102	0.0509	0.635	-0.2308	$24^3 \times 64$	0.863 72	1040	5	1.0	0.036	0.66	2.574(5)	$0.1211_{(-12)}^{(+6)}$
6.3	0.0074	0.037	0.440	-0.1205	$32^3 \times 96$	0.874 164	878	6	1.5	0.031	0.68	3.520(7)	$0.0886_{(-9)}^{(+4)}$

First, the HISQ simulations include the effects of a dynamical charm quark. We expect that the effects of dynamical charm will be very small for the quantities studied here, but with modern algorithms it is cheap to include the charm quark, and we plan to investigate quantities involving dynamical charm in the future.

Second, the one-quark-loop contributions to the perturbative calculation of the coefficients in the Symanzik improved gauge action are included. At the time the asqtad simulation program was started these corrections were not available, but they have now been computed for both the asqtad and HISQ actions, and are unexpectedly large [8].

Third, in the HISQ action the parallel transport of quark fields is done with a link that is highly smeared. Specifically, it is first smeared using a “fat7” smearing, then projected onto a unitary matrix, and then smeared again with an “asqtad” smearing [3]. The use of the asqtad smearing in the second iteration, together with the addition of the Naik term, or third-nearest-neighbor coupling, in $\not{D}$, ensures that the fermion action is formally order a^2 improved. The use of two levels of smearing produces a smooth gauge field as seen by the quarks, and this explains the reduced taste symmetry violations.

Finally, the third-nearest-neighbor term in the charm quark $\not{D}$ is modified to improve the charm quark dispersion relation [3]. These last two differences combine to make up what is usually meant by “the HISQ action,” although in principle they could be introduced independently.

Where practical, since our purpose is to compare the lattice artifacts in the two actions, we use the same analysis for the HISQ data as was used for the asqtad data.

Table I shows the parameters of the three HISQ runs used in these tests. Detailed information about the asqtad ensembles can be found in Ref. [4].

The HISQ lattices were generated using the rational hybrid Monte Carlo algorithm [10]. Issues with implementing this algorithm for the HISQ action have been discussed in Ref. [11]. We used different molecular dynamics step sizes for the gauge and fermion parts of the action, with three gauge steps for each fermion step [12].

We used the Omelyan integration algorithm in both the gauge and fermion parts [12,13]. Five pseudofermion fields were used, each with a rational function approximation for the fractional powers. The first implements the ratio of the roots of the determinants for the light and strange sea quarks to the determinant for three heavy “regulator” quarks with mass $am_r = 0.2$. That is, it corresponds to the weight $\det(M(m_l))^{1/2} \det(M(m_s))^{1/4} \det(M(m_r))^{-3/4}$. The next three pseudofermion fields each implement the force from one flavor of the regulator quark, or the fourth root of the corresponding determinant [14]. The final pseudofermion field implements the dynamical charm quark.

Rational function approximations were used for the fractional powers of the matrices [10,15]. In the molecular dynamics evolution we used a 9th order approximation for the pseudofermion field containing the light quarks, and a 7th order approximation for the three regulator fields and the charm quark pseudofermion. For the heat bath updating of the pseudofermion fields and for computing the action at the beginning and end of the molecular dynamics trajectory, we used 11th order and 9th order approximations. These approximations comfortably exceeded the required accuracy, but since a multimass conjugate gradient routine is used for the sparse matrix solutions, adding extra terms in these approximations has minimal cost.

In order to make this paper self-contained, we summarize the action in Appendix A, and discuss some algorithmic issues specific to the HISQ action in Appendixes B, C, and D.

III. AUTOCORRELATIONS IN SIMULATION TIME

Estimating statistical errors on any physical quantity requires taking into account the fact that successive sample configurations are not completely statistically independent, and calculations of statistical errors that ignore these autocorrelations are generally underestimates of the true errors. The amount of autocorrelation depends strongly on the quantity under consideration, so we present

autocorrelations for a few simple but relevant quantities. To parametrize autocorrelations we use the dimensionless coefficient

$$C_{\Delta t} = \frac{\langle x_i x_{i+\Delta t} \rangle - \langle x_i \rangle^2}{\langle x_i^2 \rangle - \langle x_i \rangle^2}, \quad (1)$$

where x_i is the measurement at simulation time i and Δt is the time separation of the two measurements. As discussed above, in these simulations successive lattices were saved at time separations $\Delta t = 5$ for the $a = 0.15$ and 0.12 fm ensembles, and $\Delta t = 6$ for the 0.09 fm ensemble. However, measurements of the plaquette and $\bar{\psi}\psi$ were made every trajectory. Note that determination of these autocorrelation coefficients is numerically difficult, even on time series of order 1000 lattices. This is partly because of the practical necessity of using the average $\langle x_i \rangle$ from our simulation, rather than the true average. (Note, however, that for the topological charge we know that the true average is zero.) Estimation of errors on these coefficients is also noisy. Here we have estimated the errors from the variance of autocorrelations measured on five separate segments of the time series, but for the central value quote the result from the full time series.

The autocorrelations can be taken into account either by blocking the data (averaging over intervals of time) and then computing the average of the blocked values, or by multiplying the error estimate ignoring autocorrelations by the factor

$$\sqrt{1 + 2 \sum_i C_i}, \quad (2)$$

with the sum suitably truncated. For complicated functions of observables a jackknife analysis can be used, and Eqs. (1) and (2) applied to the sequence of jackknife results.

We begin with the plaquette and strange-quark $\bar{\psi}\psi$, simple observables which were measured at each trajectory. The first two panels of Fig. 1 show the autocorrelation of these quantities as a function of separation in simulation time. Here $\bar{\psi}\psi$ is estimated using a single random source vector. Thus part of its variance comes from the random source, and part from the variation of the lattice. For this reason, its autocorrelation does not approach one at small time. We show the strange-quark $\bar{\psi}\psi$ because it generally shows larger autocorrelations than the light-quark $\bar{\psi}\psi$. Also, relevant to future ensembles at other light-quark masses, it will be useful to compare autocorrelations using $\bar{\psi}\psi$ at a fixed physical quark mass. These two simple quantities provide a good illustration of how autocorrelations differ among various quantities.

Table II shows these quantities at the time separation of the stored lattices, and a selection of autocorrelations of more physically relevant quantities. In particular, it contains autocorrelations of the pion and rho correlators ($\langle \pi(0)\pi(D) \rangle$ and $\langle \rho(0)\rho(D) \rangle$) at a distance D equal to the minimum distance that might be used in a mass fit, and would be one of the important contributors to the mass. This table also contains autocorrelations of single elimination jackknife measurements of the pion mass, the pion decay constant (amplitude of a pion correlator), and the rho meson mass.

The topological charge is generally expected to have a long autocorrelation time. In fact, in the continuum limit, tunnelings would be expected to be completely suppressed in a simulation algorithm where the configurations evolve continuously. Such a simulation would still give correct results in infinite volume, but would have power-law finite volume effects [16]. The right panel in Fig. 1 shows the autocorrelation of the topological charge in the $a = 0.12$ and 0.09 fm ensembles. As expected, the autocorrelation time is larger for this quantity than for the others, and is

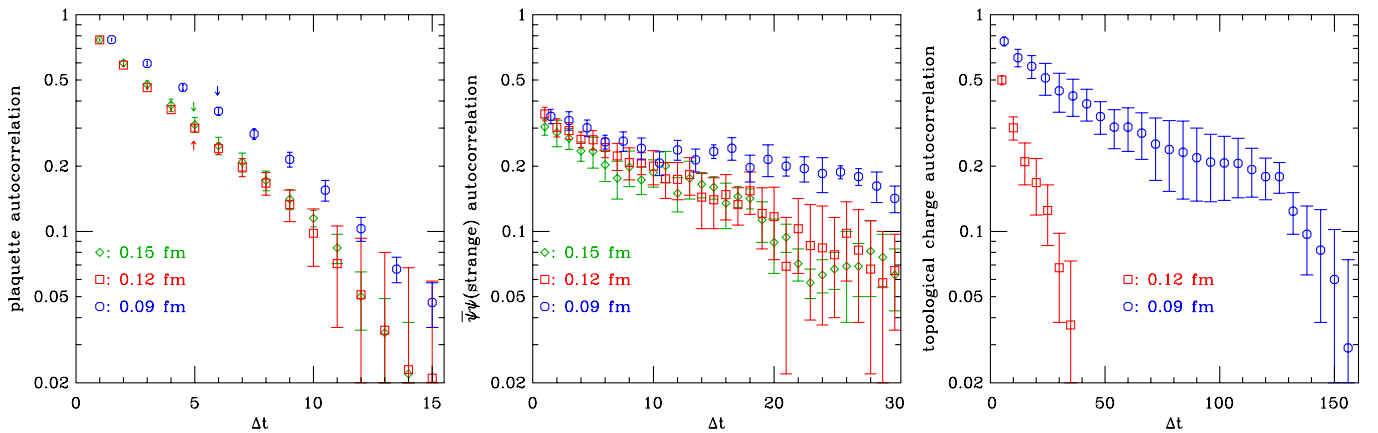


FIG. 1 (color online). Autocorrelation $C_{\Delta t}$ in simulation time of the plaquette (left panel), strange-quark $\bar{\psi}\psi$ (center panel), and topological charge (right panel). Note that the horizontal scale is different in each of the three panels. Errors on the autocorrelation were estimated by dividing the time series into five subsets and averaging the autocorrelations from each subset. The vertical arrows in the left panel indicate the time separation between stored lattices, used in computing the potential, spectrum, and other quantities.

TABLE II. Autocorrelation $C_{\Delta t}$ of various quantities between successive lattices in the ensembles. Lattices are separated by five time units for $a = 0.15$ and 0.12 fm, and by six time units for $a = 0.09$ fm. As discussed in the text, the autocorrelations for $\bar{\psi}\psi$ are between estimates made with one random source. Autocorrelations for the correlators $\langle\pi(0)\pi(D)\rangle$ and $\langle\rho(0)\rho(D)\rangle$ are given at a spatial distance D which is the minimum distance used in a typical fit for the mass. For the pion correlator these distances are $D = 15, 20$, and 30 , respectively, and for the ρ correlator they are $D = 6, 7$, and 10 , respectively. For the pion and rho mass and f_π the autocorrelations are from single elimination jackknife samples.

Operator	0.15 fm	0.12 fm	0.09 fm
$\square$	0.311(25)	0.300(10)	0.359(14)
$\bar{\psi}\psi_{\text{light}}$	0.135(24)	0.151(27)	0.192(34)
$\bar{\psi}\psi_{\text{strange}}$	0.234(38)	0.265(27)	0.259(19)
$\langle\pi(0)\pi(D)\rangle$	0.034(40)	0.084(46)	0.177(21)
$\langle\rho(0)\rho(D)\rangle$	0.055(24)	0.074(24)	0.061(18)
m_π	0.008(14)	0.182(35)	0.249(51)
f_π	0.123(21)	0.150(23)	0.184(45)
m_ρ	0.036(38)	0.045(09)	0.002(24)
Q_{topo}	...	0.500(25)	0.754(36)

much larger on the finer ensemble. The long autocorrelation time means that it will be important to check the size of finite volume effects; such runs are planned.

In the sections below, the static quark potential was computed using block sizes of 50 time units for $a = 0.15$ and 0.12 fm, and 60 time units for $a = 0.09$ fm. For the pseudoscalar meson plot, block sizes of 20 and 24 time units were used. Autocorrelations for the rho and nucleon masses are small, and were neglected here.

IV. THE STATIC QUARK POTENTIAL

Although it is not a physical observable, the potential between two infinitely heavy test quarks is well defined on the lattice and can be computed with high precision and comparatively little effort. Therefore it has become conventional in lattice simulations to use a length scale based on the static quark potential to relate lattice simulations with different couplings, and to translate the dimensionless results of lattice simulations into physical units. We generally use r_1 defined by $r_1^2 F(r_1) = -1$, where $F(r)$ is the force $-\frac{\partial V(r)}{\partial r}$. The scale r_0 defined by $r_0^2 F(r_0) = -1.65$ is also commonly used. [The idea behind scales of this form [17] is that they locate the transition region between the Coulomb potential at short distances, $r^2 F(r) = -\frac{4}{3}\alpha$, and the linear potential at long distances, $r^2 F(r) = -\sigma r^2$.]

In order to determine r_1 , we measure the static potential at discrete distances $r^2/a^2 = n_x^2 + n_y^2 + n_z^2$, and for a range of r approximately centered at r_1 , we fit it to the functional form [18]

$$V(R) = C + \frac{B}{R} + \sigma R + \lambda \left(\frac{1}{R} \Big|_{\text{lat}} - \frac{1}{R} \right). \quad (3)$$

Here $\frac{1}{R}|_{\text{lat}}$ is the the lattice Coulomb potential, $\frac{1}{R}|_{\text{lat}} = 4\pi \int \frac{d^3 p}{(2\pi)^3} D_{00}^{(0)}(p) e^{ipR}$, with $D_{00}^{(0)}(p)$ the free lattice gluon propagator calculated with the Symanzik improved gauge action, and $1/R$ is the continuum Coulomb potential.

Figure 2 shows the static quark potential at $a \approx 0.09$ fm for the HISQ ensemble and a corresponding asqtad ensemble. Overall, the two potentials are very similar. For reference, the value of r_1/a for this HISQ ensemble in Table I came from a fit to the range $\sqrt{5} \leq r/a \leq 6$, or $0.63 < r/r_1 < 1.70$. The inset in Fig. 2 makes visible some of the lattice artifacts at short distance. In particular, the HISQ point at $r/r_1 = 0.57$ and the asqtad point at 0.53 correspond to separation $(2, 0, 0)$ along a lattice axis, and are visibly displaced below the trend. Note that artifacts of this kind are not decreased with the HISQ action, and we do not expect them to be decreased. In fact, in the continuum limit we expect them to be described by Eq. (3) with $\lambda = B$. [The fit to this potential has $B = -0.441(6)$ and $\lambda = -0.52(11)$.] Artifacts like this, at fixed number of lattice spacings, simply move to $r = 0$ in the continuum limit. Also note that these artifacts diminish quickly with increasing r . For example, the HISQ point at $r/r_1 = 0.95$ is really two points, with $\vec{r}/a = (3, 0, 0)$ and $(2, 2, 1)$, and the difference between the two potential values is invisible.

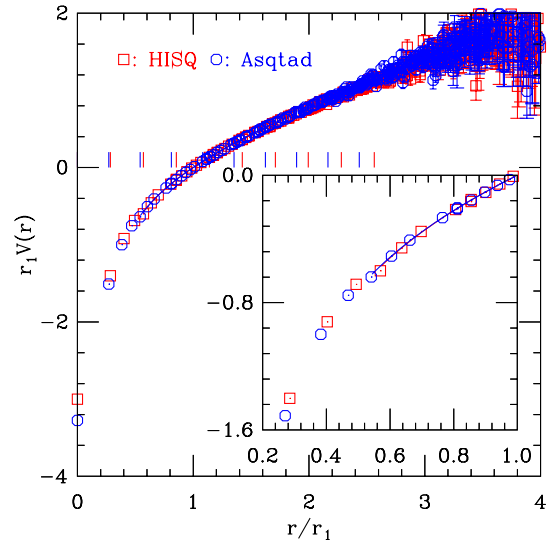


FIG. 2 (color online). The static quark potential with the HISQ and the asqtad actions. The HISQ results are from the $a \approx 0.09$ fm run, and the asqtad results are from a lattice with almost the same lattice spacing and light-quark mass about 0.2 times the correct strange-quark mass ($am_l = 0.00465$). In order to match the potentials, the plot is in units of r_1 , while rulers in units of the lattice spacing are shown at $r_1 V(r) = 0$. A constant has been added to each potential so that $V(r_1) = 0$. The solid lines (essentially superimposed) show the fit from Eq. (3) for the two runs (evaluated with λ set to zero). The inset magnifies a part of this plot at short distance to show the lattice artifacts discussed in the text.

TABLE III. Parameters of the potential fits in Fig. 2. As discussed in the text, in this comparison the fit ranges for the HISQ potential were chosen to match those used for the asqtad potential, and so these tabulated parameters differ slightly from those used in the rest of this paper. Note that the lattice mass is regularization dependent—in both of these ensembles the light-quark mass is about one-fifth of the correct strange-quark mass.

	Asqtad	HISQ
Fit range	2.01–6.5	2.01–6.5
Time separations	5–6	5–6
$10/g^2$	7.085	6.30
$am_l/am_s/am_c$	0.004 65/0.031/na	0.0074/0.037/0.440
aC	0.849(3)	0.824(3)
B	−0.432(4)	−0.450(5)
σr_1^2	0.568(6)	0.554(6)
r_1/a	3.697(7)	3.510(7)

We expect that these short-distance lattice artifacts in the static quark potential are mostly controlled by the gauge actions, which differ only in the fermion contributions to the one-loop corrections.

We do expect scaling violations proportional to a^4 and to $a^2\alpha^2$ at physical distances for both actions, and these would be visible in quantities like r_0/r_1 or $r_1\sqrt{\sigma}$. However, it is not possible to make a definitive comparison of scaling violations in these quantities between the two actions yet, since the addition of the dynamical charm quark to the HISQ simulations could also have small effects on these quantities.

For reference, Table III shows the parameters of the fits in Fig. 2, defined in Eq. (3). Note that in this figure the fitting range used for the HISQ run is the same as used for the asqtad ensemble, and so differs from that used in finding the value of r_1/a in Table I. Also note that the quantity σr_1^2 parametrizes the potential in the range around r_1 , and should not be used as a measurement of the long-distance string tension. Finally, note that since the dimensionful parameters are expressed in units of r_1 , which is found from the same fit, one relation between B and σ is automatically enforced. In Fig. 2 this constraint forces both fits to have the same slope at $r = r_1$ [since r_1 is defined by the slope (force) at this distance], and a constant was subtracted to make both fits be zero at this point.

V. SCALING TESTS

Reduction of taste splittings among the pion masses with HISQ valence quarks was demonstrated with quenched gauge fields in Refs. [1,2], and with asqtad sea quarks in Ref. [3], and there is little reason to expect it to be different with dynamical HISQ sea quarks. However, in view of the importance of this quantity, we show splittings for all of the different tastes of pions in Fig. 3, comparing results with HISQ quarks (both valence and sea) to earlier results with

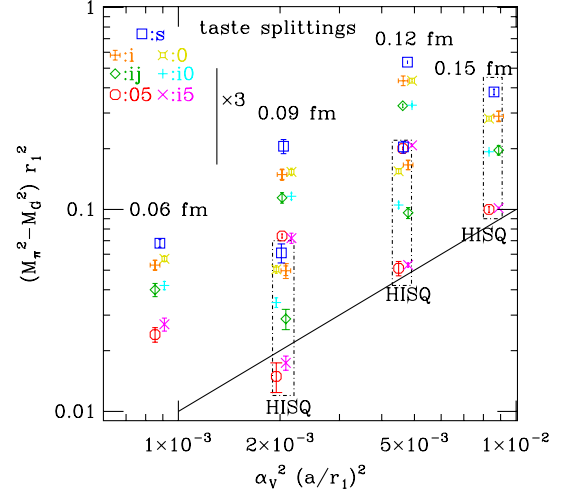


FIG. 3 (color online). Taste splittings among the pions. The asqtad results used configurations with 2 + 1 flavors of dynamical quarks, and the HISQ results 2 + 1 + 1 flavors. The quantity plotted is $r_1^2(M_\pi^2 - M_G^2)$, where M_π is the mass of the non-Goldstone pion and M_G is the mass of the Goldstone pion. Reading from top to bottom, the non-Goldstone pions are the π_s (box), π_0 (fancy box), π_i (fancy plus), π_{io} (plus), π_{ij} (diamond), π_{i5} (cross), and π_{05} (octagon). $r_1^2(M_\pi^2 - M_G^2)$ is known to be almost independent of the light-quark mass. The vertical bar at the upper left shows the size of a factor of 3, roughly the observed reduction in taste splittings, while the sloping solid line shows the theoretically expected dependence on lattice spacing. Nearly degenerate points have been shifted horizontally to improve their visibility.

asqtad quarks. In this figure, we see that the expected reduction in taste splittings happens, with roughly a factor of 3 reduction relative to asqtad calculations at the same lattice spacing.

The main purpose of this study was to see if the improvements in the action designed to reduce taste symmetry violations translate into decreased lattice spacing dependence in other quantities. We begin with the mass of the light-quark vector meson, or ρ . In Fig. 4 we show the mass of the ρ meson in units of r_1 . Here we have asqtad results for several light-quark masses at each lattice spacing, but HISQ results for only one light-quark mass. The light-quark masses themselves are regularization dependent, so to plot asqtad and HISQ results on the same footing we use the Goldstone pion mass in units of r_1 for the horizontal axis. Note that for $m_l = 0.2m_s$, the light-quark mass used in the HISQ simulations, and for the lattice sizes used here (≤ 2.9 fm), the vector meson is stable against decay to two pions. Results for the nucleon mass are similar, and are shown in Fig. 5. In Figs. 4 and 5 the HISQ masses show smaller dependence on the lattice spacing than the asqtad masses, with the same continuum limits within the statistical errors. Roughly speaking, the HISQ results are similar to the asqtad results at the next smaller lattice spacing.

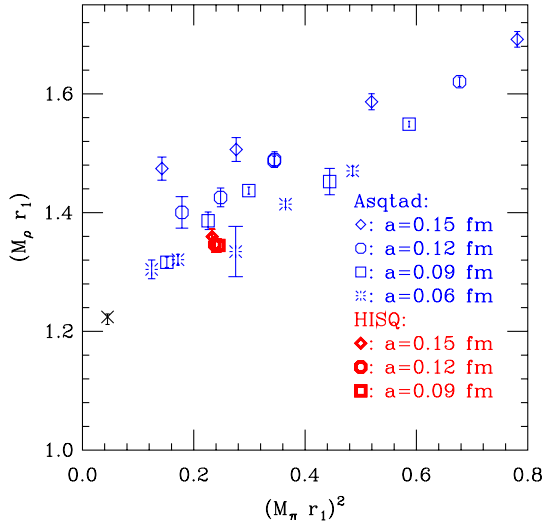


FIG. 4 (color online). Vector meson (ρ) masses in units of r_1 . Here the bold (red) points are the HISQ simulations with $m_l = 0.2m_s$, and the lighter (blue) points are asqtad results for various light-quark masses. The $a \approx 0.06$ fm asqtad point immediately to the right of the $a \approx 0.09$ fm HISQ point has been displaced to the right to make it visible. It in fact falls on top of the $a \approx 0.09$ fm HISQ point. The cross sign at lower left is the physical ρ mass. The error on the physical mass point is just the error on the physical value of r_1 .

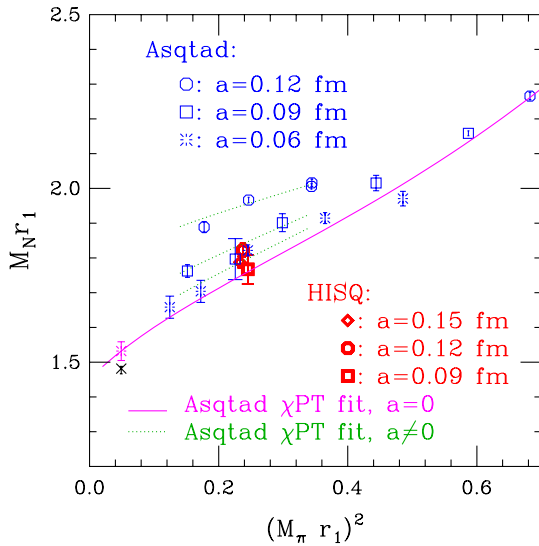


FIG. 5 (color online). Nucleon masses in units of r_1 . Here the bold (red) points are the HISQ simulations with $m_l = 0.2m_s$, and the lighter (blue) points are asqtad results for various light-quark masses. The cross at lower left is the physical nucleon mass. The solid magenta line is a continuum extrapolation of a chiral perturbation theory fit to the asqtad nucleon masses, while the dotted green lines are from the same fit at finite lattice spacing [32].

Although we have chosen to present these results as improved scaling of the ρ and nucleon masses, since we are plotting the dimensionless quantities $M_\rho r_1$ and $M_N r_1$, they could equally well be described as improved scaling of r_1 when a hadron mass is chosen to be the length standard.

The pseudoscalar meson decay constants are important for lattice determinations of Cabibbo-Kobayashi-Maskawa matrix elements, and can be computed with high precision. In fact, our current best determination of r_1 in physical units comes from matching the asqtad lattice results to the physical value of f_π . These decay constants for light quarks have been extensively studied using the asqtad ensembles [4,19]. The HPQCD Collaboration has computed these decay constants in a mixed action calculation, with HISQ valence quarks on the asqtad sea-quark ensembles, and used them in a determination of the physical value of r_1 [20]. Figure 6 shows the pseudoscalar decay constant with one of the valence quarks fixed at approximately the strange-quark mass as a function of the mass of the other valence quark. (At the physical light-quark mass, this is just f_K .) To facilitate the comparison, we have used the ratio of the light-quark mass to the corrected strange-quark mass in the corresponding ensemble for the horizontal axis. The reduction in lattice artifacts is obvious, and it can also be seen that the HISQ points lie near the continuum limit of the asqtad points. Once again, we remark that since the plotted quantity is $r_1 f_{PS}$, this could equally well be described as scaling of r_1 or scaling of f_{PS} .

The topological susceptibility is a particularly important test here, since it is computed solely from the gluon configurations that are generated, without involving HISQ or asqtad valence quarks. Therefore improvements in the scaling of the topological susceptibility directly test whether the change of the sea-quark action has the expected effect on the gluon configurations that are generated. Our technique for calculating the topological susceptibility is set out in detail in Ref. [21]. Here we just note that this technique is based on measurement of a density-density correlator, and hence is not limited by long autocorrelation times for the overall topological charge. Figure 7 shows the topological susceptibility for most of the asqtad ensembles, and HISQ results for the $a \approx 0.12$ fm and $a \approx 0.09$ fm ensembles. The HISQ point with $a \approx 0.12$ fm lies near the asqtad points with $a \approx 0.09$ fm, and the HISQ point with $a \approx 0.09$ fm is near the asqtad points with $a \approx 0.06$ fm, demonstrating a decrease in lattice artifacts. Note that the HISQ points are to the left of the corresponding asqtad points, which are indicated by arrows in the figure. This is because the horizontal axis is the mass of the taste singlet pion (the heaviest pion taste), and the reduction in taste symmetry breaking moves the points to the left. It is the movement down relative to the asqtad points that represents an improvement in the gluon configurations.

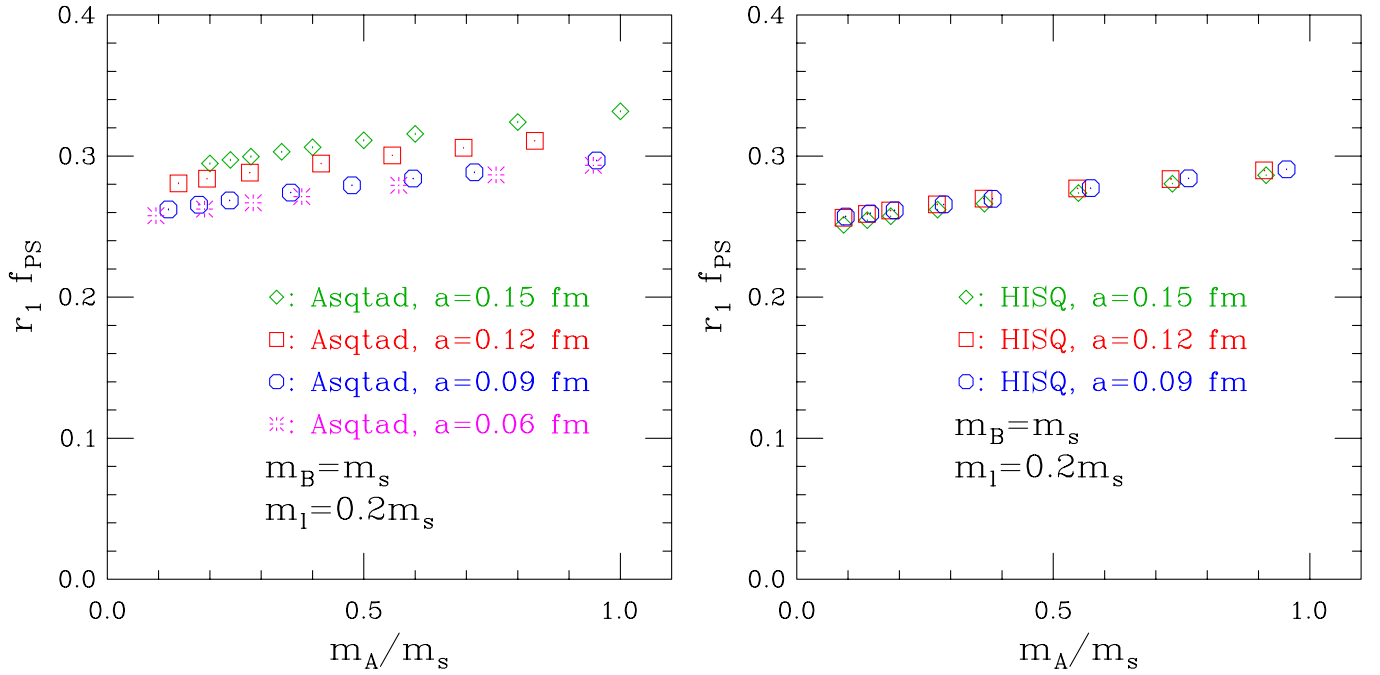


FIG. 6 (color online). Pseudoscalar decay constant. One valence-quark mass, m_A , is varied while the second is held fixed near the strange-quark mass. All ensembles used a light sea-quark mass of about 0.2 times the strange-quark mass. The left-hand panel shows asqtad results for four different lattice spacings and the right-hand panel shows HISQ results for three lattice spacings.

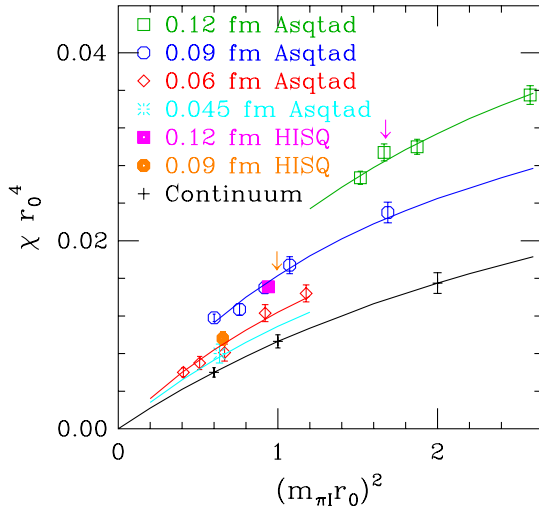


FIG. 7 (color online). The topological susceptibility. Points with the asqtad action are shown for several lattice spacings and quark masses, and the HISQ results for $a \approx 0.12$ fm and $a \approx 0.09$ fm with $m_l = 0.2m_s$. For the horizontal axis we use the mass of the taste singlet pion, since in lowest order chiral perturbation theory the topological susceptibility is a function of this mass [33]. The curves in the figure come from a chiral perturbation theory fit to the asqtad data. The asqtad results are updated from Ref. [34] and are discussed further in Refs. [4,21]. The two arrows indicate the locations of asqtad points with lattice spacing and quark mass similar to the two HISQ points. (In the case of the $a \approx 0.09$ fm HISQ point, the quark mass falls between two of the masses of the asqtad points.)

VI. USING f_{ss} TO SET THE SCALE

In Figs. 4–6 it can be seen that $r_1 f_K$ and the hadron masses in units of r_1 all increase as the lattice becomes coarser. This common dependence on lattice spacing could be absorbed into a lattice spacing dependence of r_1 . Put more simply, we could use one of these quantities to set the lattice spacing. Such a procedure has been introduced and studied by the HPQCD Collaboration in Ref. [20]. In particular, they use the decay constant of a fictitious “unmixed $\bar{s}s$ ” pseudoscalar meson, which is an isospin nonsinglet meson with both valence quarks having mass m_s , to set the scale. We call this decay constant f_{ss} . Like r_1 , f_{ss} is not a quantity that can be directly determined from experiment, and so, like r_1 , its physical value is eventually determined by matching to some precisely known quantity such as f_π or mass splittings of heavy quark mesons. In practice, the HPQCD Collaboration determines f_{ss} and the corresponding meson mass M_{ss} using a next-to-leading-order chiral fit (augmented with discretization corrections) to their lattice data, and inputs of the experimental values for f_π , f_K , M_π , and M_K . In fact, lowest order chiral perturbation theory with these experimental values alone (without lattice data) gets within $\sim 1\%$ of the HPQCD results [20]. We prefer not to input the experimental value f_K in such determinations, since we take f_K as an output of our lattice calculations that gives a result for V_{us} [4,19]. Indeed, f_π , M_π , and M_K alone are adequate for determining the physical scale and the quark masses m_l and m_s , and hence all light-quark quantities.

TABLE IV. Lattice spacings in fm from $r_1 = 0.3117$ fm, f_{ss} with asqtad valence quarks, and f_{ss} with HISQ valence quarks. The first five columns identify the ensemble by the sea-quark action, the gauge coupling $10/g^2$, and the sea-quark masses. The horizontal line separates ensembles with asqtad sea quarks (above) from those with HISQ sea quarks (below). The values for HISQ valence quarks on asqtad sea ensembles are taken from Ref. [20]. The errors on $a(r_1)$ are statistical only—they do not include the errors in $r_1 = 0.3117(6)(^{+12}_{-31})$ fm. Similarly, the errors on $a(f_{ss} - \text{asqtad})$ and $a(f_{ss} - \text{HISQ})$ for the HISQ ensembles do not include any errors in the physical value of f_{ss} . The numbers following the f_{ss} lattice spacings are the value of the valence strange-quark mass am_s at which the desired ratio is obtained. We use the values $f_{ss} = 181.5$ MeV and $f_{ss}/M_{ss} = 0.2647$ from Ref. [20].

Action	$10/g^2$	am_l	am_s	am_c	$a(r_1)$	$a(f_{ss} - \text{asqtad})$	am_s	$a(f_{ss} - \text{HISQ})$	am_s
Asqtad	6.76	0.01	0.05		0.1178(2)	0.1373(2)	0.0467	0.1264(11)	0.0553
Asqtad	7.09	0.0062	0.031		0.0845(1)	0.0905(3)	0.0286	0.0878(7)	0.0362
Asqtad	7.46	0.0036	0.018		0.0588(2)	0.0607(1)	0.0187	0.0601(5)	0.0233
Asqtad	7.81	0.0028	0.014		0.0436(2)	0.0444(1)	0.0133	0.0443(4)	0.0163
HISQ	5.80	0.013	0.065	0.838	0.1527(7)	...	...	0.1558(3)	0.0720
HISQ	6.00	0.0102	0.0509	0.635	0.1211(2)	...	...	0.1244(2)	0.0549
HISQ	6.30	0.0074	0.037	0.440	0.0884(2)	...	...	0.0900(1)	0.0374

An advantage of using f_{ss} to set the scale on a given lattice ensemble is that it can be determined to high accuracy in the simulations. However, it has the disadvantage that it depends on the choice of valence quarks, so the lattice spacing assigned to a particular ensemble will depend slightly on whether it is determined with asqtad quarks, HISQ quarks, or some other formalism.

Table IV shows the lattice spacings of the three HISQ ensembles used in this paper, and some comparable asqtad ensembles, using r_1 and f_{ss} as the length standards. For the asqtad ensembles, we show the effect of using either asqtad or HISQ valence quarks to determine the lattice spacing. Note that, as expected, the differences among the scale determinations decrease as the lattice spacing decreases. The values of f_{ss} and the corresponding

strange-quark mass am_s were determined by fitting a quadratic polynomial through masses and decay constants at valence masses equal to 1.0, 0.8, and 0.6 times the sea strange-quark mass. Table IV also shows the value of the strange-quark mass am_s given by this interpolation or extrapolation. Figure 8 shows the differences in length scale (relative to the determination from r_1) as a function of lattice spacing. In this figure it can be seen that these differences are vanishing in the expected way as the lattice spacing decreases.

In Fig. 9 we show the rho mass data from Fig. 4 replotted using f_{ss} to set the scale. Replotting the nucleon masses in Fig. 5 would produce similar results. (Of course, one could then make a plot showing the dependence of $r_1 f_{ss}$ on sea-quark mass and lattice spacing.)

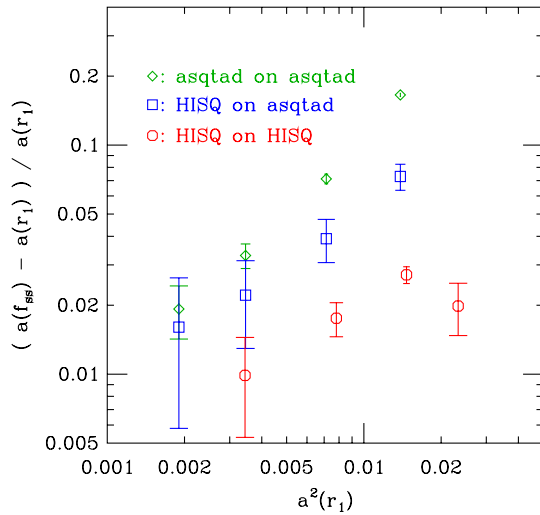


FIG. 8 (color online). Differences in determinations of the length scale using different standards. In the legend, the symbol types are labeled as “valence on sea.” The “HISQ on asqtad” points are taken from Ref. [20].

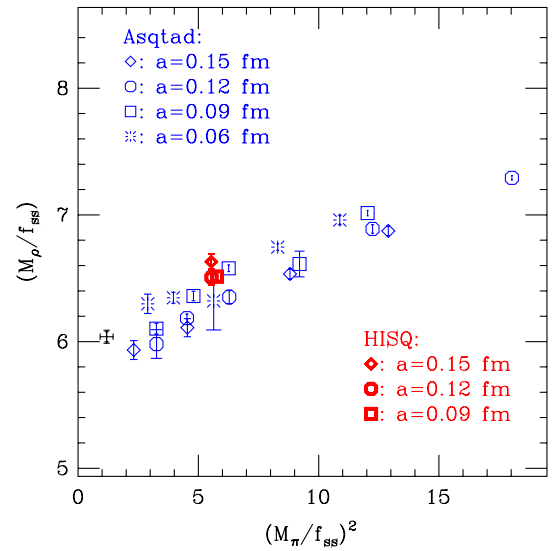


FIG. 9 (color online). Vector meson (ρ) masses in units of f_{ss} . The data and the meaning of the symbols are the same as in Fig. 4. The vertical and horizontal scales in the figure correspond to the same ranges as in Fig. 4.

VII. CONCLUSIONS

Using simulations with a fixed and unphysically large light-quark mass, we see that dimensionless ratios of several hadronic quantities show smaller dependence on lattice spacing with the HISQ action than with the asqtad action. Roughly, for the quantities that we checked, HISQ simulations at lattice spacing a appear to have similar lattice artifacts as asqtad simulations at lattice spacing $\frac{2}{3}a$, leading to substantial savings in simulation costs. This program is continuing with computations at different light sea-quark masses, so that both the extrapolation to the continuum limit and the extrapolation to the physical light-quark mass can be controlled.

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APPENDIX A: GAUGE AND FERMION ACTIONS

For completeness, we summarize the gauge and fermion actions in this appendix.

The gauge action is a tadpole-improved [22] one-loop-Symanzik-improved gauge action [23] including the effects of the quark loops in the one-loop coefficients [8]. The number of flavors n_f is set to four in these simulations.

This gauge action involves three kinds of loops: the 1×1 loop, or plaquette P , the 2×1 loop, or rectangle

R , and the twisted loop T , which traverses paths such as $+\hat{x}, +\hat{y}, +\hat{z}, -\hat{x}, -\hat{y}, -\hat{z}$. Then

$$S_g = \beta \left(C_P \sum_P \left(1 - \frac{1}{3} \text{Re Tr}(P) \right) + C_R \sum_R \left(1 - \frac{1}{3} \text{Re Tr}(R) \right) + C_T \sum_T \left(1 - \frac{1}{3} \text{Re Tr}(T) \right) \right), \quad (\text{A1})$$

where the sums run over all distinct positions and orientations of the loops. The coefficients are

$$\begin{aligned} C_P &= 1.0, \\ C_R &= \frac{-1}{20u_0^2} (1 - (0.6264 - 1.1746n_f) \ln(u_0)), \\ C_T &= \frac{1}{u_0^2} (0.0433 - 0.0156n_f) \ln(u_0). \end{aligned} \quad (\text{A2})$$

In this expression the strong coupling constant appears in the form $\alpha_s = -\ln(u_0)/1.303615$. With this normalization $\beta = \frac{10}{g^2}$. We determine the tadpole coefficient u_0 from the average plaquette, $u_0 = (\langle \text{Re Tr} P \rangle / 3)^{1/4}$.

The fermion factor in the partition function is

$$\ln(S_f) = \prod_f (\det(2\not{D} + 2m_f))^{1/4}. \quad (\text{A3})$$

The Dirac operator $\not{D}$ is constructed from smeared links. Two levels of smearing are used, with a projection onto an element of $U(3)$ after the first smearing. The fundamental gauge links are $U_\mu(x)$, the fat links after a level one fat7 smearing are $V_\mu(x)$, the reunitarized links are $W_\mu(x)$, and the fat links after level two asqtad smearing are $X_\mu(x)$. The first level smeared links V are constructed from the U as a sum over products of links along paths from x to $x + \hat{\mu}$, or parallel transports.

$$V_\mu(x) = \sum_{\text{paths}} \prod_{\text{path}} U^{(+)}(\text{path}). \quad (\text{A4})$$

Table V gives the coefficients used in the two levels of smearing. The nearest neighbor part of $\not{D}$ uses the twice-smeared links X while the third-nearest-neighbor part uses the once-smeared and unitarized links W :

$$\begin{aligned} 2\not{D}_{x,y} &= \sum_\mu \{ \delta_{x+\hat{\mu},y} X_\mu(x) - \delta_{x-\hat{\mu},y} X_\mu^\dagger(x - \hat{\mu}) \} \\ &+ (1 + \epsilon_N) \{ \delta_{x+3\hat{\mu},y} W_\mu(x) W_\mu(x + \hat{\mu}) W_\mu(x + 2\hat{\mu}) \\ &- \delta_{x-3\hat{\mu},y} W_\mu^\dagger(x - 3\hat{\mu}) W_\mu^\dagger(x - 2\hat{\mu}) W_\mu^\dagger(x - \hat{\mu}) \}. \end{aligned} \quad (\text{A5})$$

In Eq. (A5) and Table V, ϵ_N is a mass-dependent correction to the tree-level improvement of the quark dispersion relation, or the “Naik term.” This correction is negligible and set to zero for the light and strange quarks. For the charm quark we use

TABLE V. Paths and coefficients used in smearing the links. It is understood that all distinct rotations and reflections of each path are used in the action. In specifying paths in this table, directions $\hat{x}$ and $\hat{y}$, etc., are different. The multiplicity is the number of such paths contributing to a single smeared link. The first block of the table gives the coefficients used in the fat7 smearing used to construct V from U . The second block gives the coefficients in the “asqtad+” smearing used to compute X from the unitarized links W , and the final line is the coefficient of the third-nearest-neighbor term. Note that the coefficient of the “Lepage” term that corrects the form factor at small momenta is twice that of the single smearing asqtad action.

Name	Path	Multiplicity	Coefficient
Single link	$+\hat{x}$	1	$1/8$
3-staple	$+\hat{y} + \hat{x} - \hat{y}$	6	$1/16$
5-staple	$+\hat{y} + \hat{z} + \hat{x} - \hat{z} - \hat{y}$	24	$1/64$
7-staple	$+\hat{y} + \hat{z} + \hat{t} + \hat{x} - \hat{t} - \hat{z} - \hat{y}$	48	$1/384$
Single link	$+\hat{x}$	1	$1/8 + 3/4 + 1/8(1 + \epsilon_N)$
3-staple	$+\hat{y} + \hat{x} - \hat{y}$	6	$1/16$
5-staple	$+\hat{y} + \hat{z} + \hat{x} - \hat{z} - \hat{y}$	24	$1/64$
7-staple	$+\hat{y} + \hat{z} + \hat{t} + \hat{x} - \hat{t} - \hat{z} - \hat{y}$	48	$1/384$
Lepage	$+\hat{y} + \hat{y} + \hat{x} - \hat{y} - \hat{y}$	6	$-1/8$
Naik	$+\hat{x} + \hat{x} + \hat{x}$	1	$-1/24(1 + \epsilon_N)$

$$\epsilon_N = -\frac{27}{40}(am_c)^2 + \frac{327}{1120}(am_c)^4 - \frac{15\,607}{268\,800}(am_c)^6 - \frac{73\,697}{3\,942\,400}(am_c)^8. \quad (\text{A6})$$

In this expression am_c is the bare mass in the quark action, and this formula combines Eqs. (24) and (26) in Ref. [3]. The numerical values of ϵ_N used in our simulations are given in Table I.

APPENDIX B: HISQ FORCE CALCULATION DETAILS

Here we summarize the details of the HISQ force calculation. For clarity in this and the next appendixes we suppress the x dependence and the direction index in the notation of the links. Most of this material appeared earlier in Ref. [11]. For the force calculation we adopted the strategy of Refs. [24,25], in which the derivative of the smeared action is calculated by repetitive application of the chain rule:

$$\frac{\partial S_f}{\partial U} = \frac{\partial S_f}{\partial X} \frac{\partial X}{\partial W} \frac{\partial W}{\partial V} \frac{\partial V}{\partial U}, \quad (\text{B1})$$

where S_f is the fermion part of the action, U are fundamental gauge links, V , the fat links after level one fat7 smearing, W , the reunitarized links, and X , the fat links after level two asqtad smearing. In our code, for the parts that involve smearing, we follow the same procedure as for the asqtad action. This procedure is described in Refs. [26,27], so we do not repeat it here. The algorithm for the reunitarization part is detailed below.

We have chosen to project links to U(3), rather than SU(3) as in the original HPQCD/UKQCD formulation, for two reasons:

(1) SU(3) projection requires calculation of the third root of the determinant, which involves a phase that can initially be restricted to, e.g., the interval $[-\pi/3, \pi/3]$. However, during the molecular dynamics evolution, this phase has to evolve continuously (to prevent the appearance of δ -function-like forces) and may cross into $[\pi/3, 2\pi/3]$ interval, and so on. Thus, SU(3) projection requires tracking the evolution of the phase for each link during molecular dynamics.

(2) For the U(3) group, different methods of projection yield the same answer for the projected link, W .

For instance, the default method in our code is polar projection: one builds a Hermitian matrix

$$Q = V^\dagger V \quad (\text{B2})$$

and then

$$W = VQ^{-1/2} \quad (\text{B3})$$

belongs to U(3), i.e.,

$$W^\dagger W = (Q^{-1/2})^\dagger V^\dagger V Q^{-1/2} = Q^{-1/2} Q Q^{-1/2} = 1. \quad (\text{B4})$$

It is important that closed-form expressions for $Q^{-1/2}$ can be derived [28] and, thus, the whole procedure can be implemented analytically.

One may expect, given that $Q^{-1/2}$ is a singular operation, that when one of the eigenvalues of Q is close to 0, the numerical accuracy in evaluation of W becomes poor. In fact, in simulations one occasionally encounters large deviations from unitarity:

$$|W^\dagger W - 1| \sim O(1). \quad (\text{B5})$$

Such situations are rare, but the contribution of (systematic) errors of this kind can be large. Therefore, we also implemented the singular value decomposition (SVD) algorithm, which is slower, but is used only in exceptional cases. We decompose

$$V = A\Sigma B^\dagger, \quad (\text{B6})$$

$A, B \in \text{U}(3)$ and Σ is a positive, diagonal matrix. (The values on the diagonal are called the singular values of V .) Then we have, simply,

$$W = AB^\dagger. \quad (\text{B7})$$

It is easy to see that (B3) gives the same result as (B7),

$$\begin{aligned} Q &= V^\dagger V = B\Sigma A^\dagger A\Sigma B^\dagger = B\Sigma\Sigma B^\dagger \\ &= B\Sigma B^\dagger B\Sigma B^\dagger = (B\Sigma B^\dagger)^2, \\ Q^{-1/2} &= (B\Sigma B^\dagger)^{-1} = (B^\dagger)^{-1}\Sigma^{-1}B^{-1} = B\Sigma^{-1}B^\dagger, \\ W &= A\Sigma B^\dagger B\Sigma^{-1}B^\dagger = AB^\dagger, \end{aligned}$$

as it should be. The SVD algorithm of Golub and Reinsch [29] is numerically stable even in the case of exactly zero eigenvalues.

Another popular projection algorithm is “trace maximization” [30]: find $W \in \text{U}(3)$ such that it maximizes

$$\Omega = \text{Re Tr}\{V^\dagger W\}. \quad (\text{B8})$$

Let us again use SVD on V :

$$V = A\Sigma B^\dagger \Rightarrow \Omega = \text{Re Tr}\{B\Sigma A^\dagger W\} = \text{Re Tr}\{\Sigma A^\dagger WB\}. \quad (\text{B9})$$

Since Σ is positive, clearly Ω is maximized when

$$A^\dagger WB = 1 \Rightarrow W = AB^\dagger \quad (\text{B10})$$

and we arrive at (B7) again. In the $\text{SU}(3)$ case an extra phase present in (B9) would lead to W different from (B7). To summarize, we use the polar projection (B3) replaced by SVD if small eigenvalues of Q are encountered.

Appendix C gives the details of calculation of $Q^{-1/2}$ and its derivative $\partial Q^{-1/2}/\partial V$ within the approach of Refs. [28,31] based on the Cayley-Hamilton theorem.

Let us now turn to the calculation of the force. During the molecular dynamics evolution, one encounters (more often on coarser ensembles) matrices V that have small eigenvalues. Let us consider the $\text{U}(1)$ group for simplicity. Then V is just an arbitrary complex number $V = re^{i\theta}$. The projection onto $\text{U}(1)$ is $W = e^{i\theta}$. The derivative that enters the force calculation is

$$\frac{\partial W}{\partial V} \equiv \left(\frac{\partial W}{\partial V} \right)_{V^\dagger} = \frac{\partial(W, V^\dagger)}{\partial(V, V^\dagger)} = \frac{\partial(W, V^\dagger)}{\partial(r, \theta)} \frac{\partial(r, \theta)}{\partial(V, V^\dagger)} = \frac{1}{2r}. \quad (\text{B11})$$

Thus the derivative is inversely proportional to the magnitude of V , or, in the $\text{U}(3)$ case, to the smallest singular

value of V (or eigenvalue of Q), which is not protected from being zero. Thus, on rare occasions one has to deal with exceptionally large forces that give large contributions to the action, but originate from a single link. In Fig. 10 we show the evolution of the minimal $\det|V|$ over the lattice and maximal value of the norm of the fermion force on a logarithmic scale. One can easily see the correlation: the lower $\det|V|$, the higher the force.

To circumvent this problem we introduce a “cutoff” in the force calculation by replacing

$$W = VQ^{-1/2} \rightarrow W = V(Q + \delta I)^{-1/2}, \quad (\text{B12})$$

where I is the unit matrix, whenever the smallest eigenvalue of Q is less than δ . In the ensembles used in this paper we set $\delta = 5 \times 10^{-5}$. In tuning δ , we weigh two competing issues: the value of δ should be large enough to suppress an exceptional contribution from a link, but small enough not to modify too many forces on the lattice. If δ is too large, the evolution will be smooth, but the fluctuation of the action will be large, usually leading to rejection of the trajectory. Note that we modify W only in the force calculation, and we use the original Eq. (B3), or Eq. (B7) for nearly singular matrices, to calculate the action at the accept/reject step. That is, the modification (B12) amounts to using a different guiding Hamiltonian during the

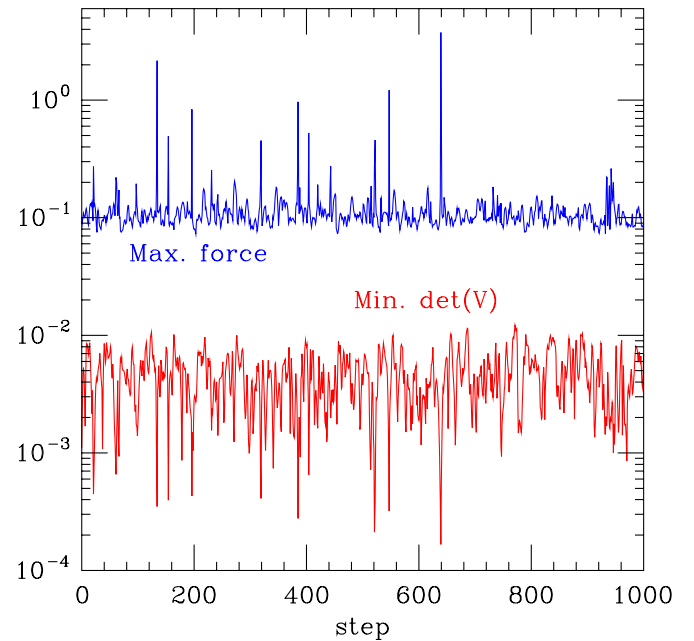


FIG. 10 (color online). Time history of the maximum (over lattice sites) magnitude of the fermion force and the minimum determinant of the fattened links after the first level of smearing (V). This exploratory run was done on a $20^3 \times 64$ lattice at $\beta = 6.75$, $am_l = 0.2am_s$, $am_s = 0.05$, $am_c = 0.6$, and $u_0 = 0.9$. This approximately corresponds to the $a \approx 0.12$ fm ensemble in Table I at $\beta = 6.0$. The difference in β is due to the use of a different gauge action in the earlier studies.

evolution, while the Metropolis step ensures the desired distribution.

APPENDIX C: ALGEBRA FOR REUNITARIZED LINKS AND THEIR DERIVATIVES

To make this presentation self-contained we include Eqs. (C1)–(C11) from Hasenfratz, Hoffmann, and Schaefer [28], preserving the notation of the original.

The inverse square root of a nonsingular matrix Q entering Eq. (B3) is given by the Cayley-Hamilton theorem as a polynomial of Q :

$$Q^{-1/2} = f_0 + f_1 Q + f_2 Q^2. \quad (C1)$$

Since Q is Hermitian, it has nonnegative eigenvalues that can be found by solving the characteristic equation

$$g^3 - c_0 g^2 - \left(c_1 - \frac{1}{2} c_0^2\right) g - \left(c_2 - c_0 c_1 + \frac{1}{6} c_0^3\right) = 0, \quad (C2)$$

where

$$c_n = \frac{1}{n+1} \text{tr} Q^{n+1}, \quad n = 0, 1, 2. \quad (C3)$$

The solution of the cubic equation (C2) is

$$g_n = \frac{c_0}{3} + 2\sqrt{S} \cos\left(\frac{\theta}{3} + (n-1)\frac{2\pi}{3}\right), \quad n = 0, 1, 2, \quad (C4)$$

where

$$S = \frac{c_1}{3} - \frac{c_0^2}{18}, \quad R = \frac{c_2}{2} - \frac{c_0 c_1}{3} + \frac{c_0^3}{27}, \quad (C5)$$

$$\theta = \arccos\left(\frac{R}{S^{3/2}}\right).$$

It is convenient to define the symmetric polynomials of the square roots of the eigenvalues

$$u = \sqrt{g_0} + \sqrt{g_1} + \sqrt{g_2},$$

$$v = \sqrt{g_0 g_1} + \sqrt{g_0 g_2} + \sqrt{g_1 g_2}, \quad w = \sqrt{g_0 g_1 g_2}. \quad (C6)$$

In the diagonalized form the expression (C1) can be rewritten as an equation for f_i

$$\begin{pmatrix} 1 & g_0 & g_0^2 \\ 1 & g_1 & g_1^2 \\ 1 & g_2 & g_2^2 \end{pmatrix} \begin{pmatrix} f_0 \\ f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} g_0^{-1/2} \\ g_1^{-1/2} \\ g_2^{-1/2} \end{pmatrix} \quad (C7)$$

which has the solution

$$f_0 = \frac{-w(u^2 + v) + uv^2}{w(uv - w)}, \quad f_1 = \frac{-w - u^3 + 2uv}{w(uv - w)},$$

$$f_2 = \frac{u}{w(uv - w)}. \quad (C8)$$

The derivative $\partial f_i / \partial c_j$ can be written as

$$B_{ij} \equiv \frac{\partial f_i}{\partial c_j} = \sum_{k=0}^2 \frac{\partial f_i}{\partial g_k} \frac{\partial g_k}{\partial c_j}. \quad (C9)$$

After rescaling (C9) by the common denominator

$$C_{ij} \equiv dB_{ij}, \quad d = 2w^3(uv - w)^3, \quad (C10)$$

a closed-form expression for the symmetric matrix C_{ij} has been derived in Ref. [28]:

$$C_{00} = -w^3 u^6 + 3vw^3 u^4 + 3v^4 w u^4 - v^6 u^3 - 4w^4 u^3$$

$$- 12v^3 w^2 u^3 + 16v^2 w^3 u^2 + 3v^5 w u^2 - 8vw^4 u$$

$$- 3v^4 w^2 u + w^5 + v^3 w^3,$$

$$C_{01} = -w^2 u^7 - v^2 w u^6 + v^4 u^5 + 6vw^2 u^5 - 5w^3 u^4$$

$$- v^3 w u^4 - 2v^5 u^3 - 6v^2 w^2 u^3 + 10vw^3 u^2$$

$$+ 6v^4 w u^2 - 3w^4 u - 6v^3 w^2 u + 2v^2 w^3,$$

$$C_{02} = w^2 u^5 + v^2 w u^4 - v^4 u^3 - 4vw^2 u^3 + 4w^3 u^2$$

$$+ 3v^3 w u^2 - 3v^2 w^2 u + vw^3,$$

$$C_{11} = -w u^8 - v^2 u^7 + 7vw u^6 + 4v^3 u^5 - 5w^2 u^5$$

$$- 16v^2 w u^4 - 4v^4 u^3 + 16vw^2 u^3 - 3w^3 u^2$$

$$+ 12v^3 w u^2 - 12v^2 w^2 u + 3vw^3,$$

$$C_{12} = w u^6 + v^2 u^5 - 5vw u^4 - 2v^3 u^3 + 4w^2 u^3$$

$$+ 6v^2 w u^2 - 6vw^2 u + w^3,$$

$$C_{22} = -w u^4 - v^2 u^3 + 3vw u^2 - 3w^2 u. \quad (C11)$$

In the following, differentiation with respect to V at fixed $V^\dagger$ is always assumed. We use explicit color indices to show how different contractions and direct products of matrices are built.

The derivatives that enter in the calculation of the fermion force are

$$\frac{\partial W_{ij}}{\partial V_{kl}} = \frac{\partial (V_{im} (Q^{-1/2})_{mj})}{\partial V_{kl}}$$

$$= \delta_{ik} (Q^{-1/2})_{lj} + V_{im} \frac{\partial (Q^{-1/2})_{mj}}{\partial V_{kl}}, \quad (C12)$$

$$\frac{\partial W_{ij}^\dagger}{\partial V_{kl}} = \frac{\partial ((Q^{-1/2})_{im} V_{mj}^\dagger)}{\partial V_{kl}} = \frac{\partial (Q^{-1/2})_{im}}{\partial V_{kl}} V_{mj}^\dagger. \quad (C13)$$

Also,

$$\frac{\partial Q_{ij}}{\partial V_{kl}} = V_{ik}^\dagger \delta_{lj}. \quad (C14)$$

The central component of the calculation is

$$\begin{aligned}
\frac{\partial(Q^{-1/2})_{ij}}{\partial Q_{pq}} &= \frac{\partial}{\partial Q_{pq}}(f_0\delta_{ij} + f_1Q_{ij} + f_2(Q^2)_{ij}) \\
&= \frac{\partial f_0}{\partial Q_{pq}}\delta_{ij} + \frac{\partial f_1}{\partial Q_{pq}}Q_{ij} + f_1\delta_{ip}\delta_{qj} \\
&\quad + \frac{\partial f_2}{\partial Q_{pq}}(Q^2)_{ij} + f_2(\delta_{ip}Q_{qj} + Q_{ip}\delta_{qj}). \quad (\text{C15})
\end{aligned}$$

From the definition (C3) it follows that $\partial c_n/\partial Q_{pq} = (Q^n)_{pq}$. Then

$$\frac{\partial f_k}{\partial Q_{pq}} = \sum_{n=0}^2 \frac{\partial f_k}{\partial c_n} \frac{\partial c_n}{\partial Q_{pq}} = \sum_{n=0}^2 B_{kn}(Q^n)_{pq}. \quad (\text{C16})$$

We define

$$P_{qp} \equiv \frac{\partial f_0}{\partial Q_{pq}} = B_{00}\delta_{qp} + B_{01}Q_{qp} + B_{02}(Q^2)_{qp}, \quad (\text{C17})$$

$$R_{qp} \equiv \frac{\partial f_1}{\partial Q_{pq}} = B_{10}\delta_{qp} + B_{11}Q_{qp} + B_{12}(Q^2)_{qp}, \quad (\text{C18})$$

$$S_{qp} \equiv \frac{\partial f_2}{\partial Q_{pq}} = B_{20}\delta_{qp} + B_{21}Q_{qp} + B_{22}(Q^2)_{qp}. \quad (\text{C19})$$

Substituting (C17)–(C19) into (C15) and Eq. (C15) in (C12) and (C13) we obtain the final result

$$\begin{aligned}
\frac{\partial W_{ij}}{\partial V_{kl}} &= \delta_{ik}(Q^{-1/2})_{lj} + [f_1(VV^\dagger)_{ik} + f_2(VQV^\dagger)_{ik}]\delta_{lj} \\
&\quad + f_2(VV^\dagger)_{ik}Q_{lj} + V_{ij}(PV^\dagger)_{lk} + (VQ)_{ij}(RV^\dagger)_{lk} \\
&\quad + (VQ^2)_{ij}(SV^\dagger)_{lk}, \quad (\text{C20})
\end{aligned}$$

$$\begin{aligned}
\frac{\partial W_{ij}^\dagger}{\partial V_{kl}} &= [f_1V_{ik}^\dagger + f_2(QV^\dagger)_{ik}]V_{lj}^\dagger + f_2V_{ik}^\dagger(QV^\dagger)_{lj} \\
&\quad + V_{ij}^\dagger(PV^\dagger)_{lk} + (QV^\dagger)_{ij}(RV^\dagger)_{lk} \\
&\quad + (Q^2V^\dagger)_{ij}(SV^\dagger)_{lk}. \quad (\text{C21})
\end{aligned}$$

The calculation of the fermion force from the reunited links proceeds as follows:

- (1) The eigenvalues of the Hermitian matrix Q are calculated with Eq. (C4).
- (2) $\det|Q|$ is compared with the product $g_0g_1g_2$. If the relative error is larger than 10^{-8} or any eigenvalue is smaller than 10^{-8} the singular value decomposition of V is performed and the eigenvalues are set to

$$g_i = \sigma_i^2, \quad i = 0, 1, 2, \quad (\text{C22})$$

where σ_i are the diagonal elements of the matrix Σ in Eq. (B6).

- (3) Additionally, if any of the eigenvalues is smaller than (an adjustable parameter) $\delta = 5 \times 10^{-5}$, the eigenvalues are modified to

$$g_i \rightarrow g_i + \delta. \quad (\text{C23})$$

[This corresponds to the force cutoff in Eq. (B12).]

- (4) With these eigenvalues the coefficients f_i and the elements B_{ij} are calculated from Eqs. (C8) and (C11).
- (5) Finally, the force is calculated from Eqs. (C20) and (C21).

In the MILC code we have also implemented two other methods for calculating $Q^{-1/2}$ and its derivative:

- (1) a rational function approximation,
- (2) an iterative evaluation of $Q^{-1/2}$ with the derivative replaced by finite difference.

We found that the analytic evaluation via Eqs. (C20) and (C21) is superior to the other methods due to its higher precision and speed.

APPENDIX D: TREATMENT OF THE HISQ CHARM QUARK

The tree-level discretization errors are $O((ap_\mu)^4)$ and are negligible for light quarks. However, at the lattice spacings listed in Table I, the charm quark mass is in the range $am_c \sim 0.4$ – 0.8 and therefore the discretization errors are larger. The leading tree-level $O((am_c)^4)$ error can be removed by retuning the coefficient of the third-nearest-neighbor (Naik) term [3], using the expansion in Eq. (A6). As can be seen from Table I, at the finest lattice, $a \approx 0.09$ fm, it is quite small, $\epsilon_N = -0.120471$. The effect of the correction in Eq. (A6) has been studied in Ref. [3]. To check the quality of charm quark physics in our ensembles, we computed the speed of light for the η_c meson by calculating its propagator at several nonzero momenta. The result is shown in Fig. 11, where

$$c^2(p) = \frac{E^2(p) - E^2(0)}{p^2} \quad (\text{D1})$$

and the momenta are rescaled by the lattice size L_s :

$$n^2 = p^2 \left(\frac{L_s}{2\pi} \right)^2. \quad (\text{D2})$$

For the finest $a \approx 0.09$ fm ensemble the error in the dispersion relation is below 2%. As expected, these η_c dispersion relations are very similar to those found for HISQ valence quarks on asqtad sea quarks, shown in Table V of Ref. [3].

For dynamical simulations, the mass-dependent correction to the Naik term requires the use of different sets of smeared links for light quarks and the charm quark. Since the difference in the Naik term enters at the second level of smearing, it is advantageous to regroup the force

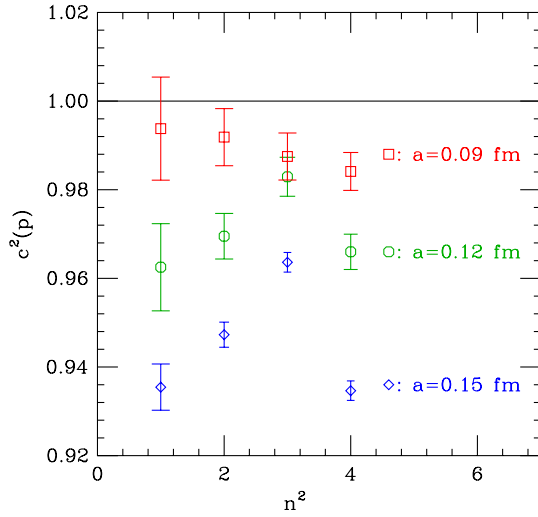


FIG. 11 (color online). The speed of light for the η_c meson calculated at several values of momenta.

calculation as described in the following. Let $X^{(0)}$ denote the fat links after level two asqtad smearing for the light quarks, for which ϵ_N is set to zero, and $X^{(c)}$ denote the fat links for the charm quark. Then the fat links for the charm quark can be written as

$$X^{(c)} = X^{(0)} + \epsilon_N \Delta X, \quad (D3)$$

where ΔX contains only one-link and three-link paths. (This can be easily seen from Table V.) The derivative is

$$\frac{\partial X^{(c)}}{\partial W} = \frac{\partial X^{(0)}}{\partial W} + \epsilon_N \frac{\partial \Delta X}{\partial W}. \quad (D4)$$

The fermion force in Eq. (B1) contains contributions from the light (u , d , and s) quarks, and from the charm quark.

$$\frac{\partial S_f}{\partial U} = \frac{\partial S_f}{\partial X^{(0)}} \frac{\partial X^{(0)}}{\partial W} \frac{\partial W}{\partial V} \frac{\partial V}{\partial U} + \frac{\partial S_f}{\partial X^{(c)}} \frac{\partial X^{(c)}}{\partial W} \frac{\partial W}{\partial V} \frac{\partial V}{\partial U}. \quad (D5)$$

The calculation of the force for multiply smeared actions proceeds from the last level of smearing to the first one. Therefore, operations with $X^{(0)}$ and $X^{(c)}$ links are done first and can be combined before the reunitarization part:

$$\begin{aligned} \frac{\partial S_f}{\partial U} &= \left(\frac{\partial S_f}{\partial X^{(0)}} \frac{\partial X^{(0)}}{\partial W} + \frac{\partial S_f}{\partial X^{(c)}} \frac{\partial X^{(c)}}{\partial W} \right) \frac{\partial W}{\partial V} \frac{\partial V}{\partial U} \\ &= \left(\left(\frac{\partial S_f}{\partial X^{(0)}} + \frac{\partial S_f}{\partial X^{(c)}} \right) \frac{\partial X^{(0)}}{\partial W} + \epsilon_N \frac{\partial S_f}{\partial X^{(c)}} \frac{\partial \Delta X}{\partial W} \right) \frac{\partial W}{\partial V} \frac{\partial V}{\partial U}. \end{aligned} \quad (D6)$$

After the $\partial \Delta X / \partial W$ contribution is separated, the number of operations needed for the HISQ fermion force is reduced to slightly more than twice the number needed for the asqtad fermion force. This is because the most time-consuming part of the calculation is related to 3-, 5-, and 7-staple paths that have high multiplicity. In our final form (D6) they are present only in $\partial X^{(0)} / \partial W$ and $\partial V / \partial U$.

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- [1] E. Follana *et al.*, Nucl. Phys. B, Proc. Suppl. **129-130**, 447 (2004).
 - [2] E. Follana *et al.*, Nucl. Phys. B, Proc. Suppl. **129-130**, 384 (2004).
 - [3] E. Follana *et al.* (HPQCD Collaboration and UKQCD Collaboration), Phys. Rev. D **75**, 054502 (2007).
 - [4] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010).
 - [5] C. T. H. Davies *et al.*, Proc. Sci., LAT2006 (2006) 082 [arXiv:hep-lat/0610110].
 - [6] E. Follana, C. T. H. Davies, G. P. Lepage, and J. Shigemitsu, Phys. Rev. Lett. **100**, 062002 (2008).
 - [7] C. T. H. Davies *et al.*, Proc. Sci., LAT2008 (2008) 118 [arXiv:0810.3548].
 - [8] Zh. Hao *et al.*, Phys. Rev. D **76**, 034507 (2007); A. Hart, G. von Hippel, and R. R. Horgan, Phys. Rev. D **79**, 074008 (2009).
 - [9] A. Bazavov *et al.*, Proc. Sci., LAT2009 (2009) 079 [arXiv:0910.3618].
 - [10] M. A. Clark and A. D. Kennedy, Nucl. Phys. B, Proc. Suppl. **129-130**, 850 (2004); Phys. Rev. D **75**, 011502 (2007); Phys. Rev. Lett. **98**, 051601 (2007).
 - [11] A. Bazavov *et al.* (MILC Collaboration), Proc. Sci., LATTICE2008 (2008) 033 [arXiv:0903.0874]; ,LAT2009 (2009) 123 [arXiv:0911.0869].
 - [12] J. C. Sexton and D. H. Weingarten, Nucl. Phys. **B380**, 665 (1992).
 - [13] I. P. Omelyan, I. M. Mryglod, and R. Folk, Phys. Rev. E **65**, 056706 (2002); T. Takaishi and Ph. de Forcrand, Phys. Rev. E **73**, 036706 (2006).
 - [14] M. Hasenbusch, Phys. Lett. B **519**, 177 (2001); M. Hasenbusch and K. Jansen, Nucl. Phys. **B659**, 299 (2003).
 - [15] The rational function approximations were computed by a code derived from one written by Mike Clark. M. A. Clark (private communication).
 - [16] H. Leutwyler and A. V. Smilga, Phys. Rev. D **46**, 5607 (1992).
 - [17] R. Sommer, Nucl. Phys. **B411**, 839 (1994).

- [18] S. P. Booth *et al.* (UKQCD Collaboration), *Phys. Lett. B* **294**, 385 (1992).
- [19] C. Aubin *et al.* (MILC Collaboration), *Phys. Rev. D* **70**, 114501 (2004); C. Bernard *et al.* (MILC Collaboration), *Proc. Sci.*, LAT2005 (2006) 025 [[arXiv:hep-lat/0509137](#)]; LAT2006 (2006) 163 [[arXiv:hep-lat/0609053](#)]; LAT2007 (2007) 090 [[arXiv:0710.1118](#)]; , [arXiv:0911.0472](#) [*Proc. Sci.*, LAT2009 (to be published)]; LAT2009 (2009) 279 [[arXiv:0910.3618](#)]; CD09 (2009) 007 [[arXiv:0910.2966](#)].
- [20] C. T. H. Davies *et al.* (HPQCD Collaboration), *Phys. Rev. D* **81**, 034506 (2010).
- [21] A. Bazavov *et al.*, *Phys. Rev. D* **81**, 114501 (2010).
- [22] G. P. Lepage and P. B. Mackenzie, *Phys. Rev. D* **48**, 2250 (1993).
- [23] K. Symanzik, in *Recent Developments in Gauge Theories*, edited by G. 't Hooft *et al.* (Plenum Press, New York, 1980), p. 313; *Nucl. Phys.* **B226**, 187 (1983); M. Lüscher and P. Weisz, *Phys. Lett.* **158B**, 250 (1985); *Commun. Math. Phys.* **97**, 59 (1985); M. G. Alford *et al.*, *Phys. Lett. B* **361**, 87 (1995).
- [24] W. Kamleh, D. B. Leinweber, and A. G. Williams, *Phys. Rev. D* **70**, 014502 (2004).
- [25] K. Y. Wong and R. M. Woloshyn, *Proc. Sci.*, LAT2007 (2007) 047 [[arXiv:0710.0737](#)].
- [26] K. Orginos and D. Toussaint, *Phys. Rev. D* **59**, 014501 (1998).
- [27] M. A. Clark, A. D. Kennedy, and Z. Sroczynski, *Nucl. Phys. B, Proc. Suppl.* **140**, 835 (2005).
- [28] A. Hasenfratz, R. Hoffmann, and S. Schaefer, *J. High Energy Phys.*, **05** (2007) 029.
- [29] G. H. Golub and C. Reinsch, *Numer. Math.* **14**, 403 (1970).
- [30] G. S. Bali and K. Schilling, *Phys. Rev. D* **46**, 2636 (1992).
- [31] C. Morningstar and M. J. Peardon, *Phys. Rev. D* **69**, 054501 (2004).
- [32] C. Bernard *et al.*, *Proc. Sci.*, LATTICE2007 (2007) 137 [[arXiv:0711.0021](#)].
- [33] C. Aubin and C. Bernard, *Phys. Rev. D* **68**, 034014 (2003); B. Billeter, C. E. DeTar, and J. Osborn, *Phys. Rev. D* **70**, 077502 (2004).
- [34] C. Bernard *et al.*, *Proc. Sci.*, LAT2007 (2007) 310 [[arXiv 0710.3124](#)].

$B_s \rightarrow D_s/B \rightarrow D$ semileptonic form-factor ratios and their application to $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-)$

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We calculate form-factor ratios between the semileptonic decays $\bar{B}^0 \rightarrow D^+ \ell^- \bar{\nu}$ and $\bar{B}_s^0 \rightarrow D_s^+ \ell^- \bar{\nu}$ with lattice QCD. These ratios are a key theoretical input in a new strategy to determine the fragmentation fractions of neutral B decays, which are needed for measurements of $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-)$. We use the MILC ensembles of gauge configurations with $2 + 1$ flavors of sea-quarks at two s of approximately 0.12 fm and 0.09 fm. We use the model-independent z parametrization to extrapolate our simulation results at small recoil toward maximum recoil. Our results for the form-factor ratios are $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2) = 1.046(44)_{\text{stat}}(15)_{\text{syst}}$ and $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_\pi^2) = 1.054(47)_{\text{stat}}(17)_{\text{syst}}$. In contrast to a QCD sum-rule calculation, no significant departure from U -spin ($d \leftrightarrow s$) symmetry is observed.

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I. INTRODUCTION

Recently there has been increasing interest in the rare decay $B_s^0 \rightarrow \mu^+ \mu^-$ which, as a flavor-changing neutral-current process, is forbidden at tree level in the standard model (SM). At the loop level, it can be mediated by weak bosons through penguin or box diagrams. With a nonperturbative (lattice QCD) calculation of the bag parameter B_{B_s} , the branching fraction has been predicted to be [1,2]

$$\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-) = 3.2(2) \times 10^{-9}. \quad (1.1)$$

Several new physics models would enhance the decay rate [3–7], and, hence, observation of this process could potentially reveal physics beyond the SM. Recently, several experiments [8–15] have published upper limits on this branching fraction, which we have compiled in Fig. 1. Moreover, CDF [11] reports an excess such that $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-) = 18_{-9}^{+11} \times 10^{-9}$ or a two-sided 90%

confidence interval, $4.6 \times 10^{-9} < \text{BR}(B_s^0 \rightarrow \mu^+ \mu^-) < 39 \times 10^{-9}$, lying above the SM prediction, Eq. (1.1). CMS and LHCb, however, set upper limits that restrict the CDF region. As statistics accumulate, especially at LHCb, a definitive measurement at the SM rate or higher seems likely soon.

At a hadron collider, the extraction of $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-)$ relies on normalization channels such as $B_u^+ \rightarrow J/\psi K^+$, $B_d^0 \rightarrow K^+ \pi^-$ and $B_s^0 \rightarrow J/\psi \phi$ [16], through relations of the form

$$\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-) = \text{BR}(B_q \rightarrow X) \frac{f_q}{f_s} \frac{\epsilon_X}{\epsilon_{\mu\mu}} \frac{N_{\mu\mu}}{N_X}, \quad (1.2)$$

where ϵ and N are, respectively, the detector efficiencies and the numbers of events. The fragmentation fractions f_q ($q = u, d, s$ or Λ) denote the probability that a b quark hadronizes into a B_q meson or a Λ_b baryon. The fragmentation fractions f_q may depend on the environment, so they are best measured *in situ* in each experiment. Thus,

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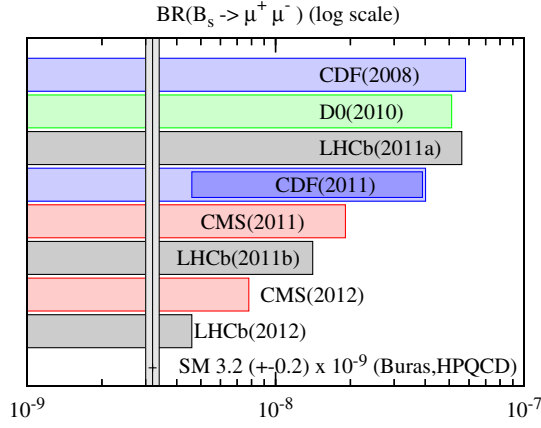


FIG. 1 (color online). Comparison of the (most recent) measurements from CDF [8,11], DØ [9], CMS [12,14], and LHCb [10,13,15] with the SM prediction [1,2] shown as a vertical band. The filled bars show the measured bounds of the branching ratio with a 95% confidence. In the fourth bar, the inner box shows the two-sided 90% bound from CDF [11]. Two results from the LHCb in 2011 are distinguished as “2011a” [10] and “2011b” [13].

improving the determination of the fragmentation ratio f_s/f_d will tighten the limits and increase the significance of measurements.

The quantity f_s/f_d has generally been determined from semileptonic decays [17], an approach that LHCb has newly refined [18]. Recently, Fleischer, Serra, and Tuning proposed two approaches based on measuring the ratio relative to nonleptonic decays $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-) / \text{BR}(\bar{B}^0 \rightarrow D^+ K^-)$ [19] or $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-) / \text{BR}(\bar{B}^0 \rightarrow D^+ \pi^-)$ [20]. An important ingredient in both approaches is the approximate factorization of the nonleptonic decay amplitudes, which relies on the corrections to naive factorization of the light-meson in the final-state being small and calculable [21]. The $D^+ K^-$ method is favored in this regard, because it receives contributions only from color-allowed tree-diagram-like topologies which yield smaller nonfactorizable effects [20].

The ratio $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-) / \text{BR}(\bar{B}^0 \rightarrow D^+ K^-)$ is related to f_s/f_d by analogy with Eq. (1.2). Via factorization, the amplitudes for these nonleptonic processes can be expressed as a product of the light-meson decay constant and a semileptonic form factor for $B_{(s)} \rightarrow D_{(s)} \ell \nu$. This leads to a way to measure f_s/f_d [19,22]:

$$\frac{f_s}{f_d} = 0.0743 \times \frac{\tau_{B^0}}{\tau_{B_s^0}} \times \left[\frac{\epsilon_{DK}}{\epsilon_{D_s\pi}} \frac{N_{D_s\pi}}{N_{DK}} \right] \times \frac{1}{\mathcal{N}_a \mathcal{N}_F}, \quad (1.3)$$

where τ denotes lifetimes, and the number 0.0743 is a product of ratios of well-known quantities such as the light-meson decay constants, Cabibbo-Kobayashi-Maskawa matrix elements and kinematic factors. The factorization is parametrized by [19]

$$\mathcal{N}_a = \left[\frac{a_1^{(s)}(D_s^+ \pi^-)}{a_1^{(d)}(D^+ K^-)} \right]^2, \quad (1.4)$$

$$\mathcal{N}_F = \left[\frac{f_0^{(s)}(M_\pi^2)}{f_0^{(d)}(M_K^2)} \right]^2, \quad (1.5)$$

where $a^{(q)}$ is a factor accounting for the deviation from the naive factorization and $f_0(q^2)$ is a form factor for the corresponding semileptonic decay.

The hadronic method relies on theoretical inputs for $\mathcal{N}_a$ and $\mathcal{N}_F$. In the limit of exact U -spin symmetry (namely the exchange of s and d quarks throughout the process), both reduce to 1. Fleischer, Serra, and Tuning expect the U -spin breaking $|\mathcal{N}_a - 1|$ “to be at most a few percent” [20,21]. Based on an estimate from QCD sum rules [23], they quote either $\mathcal{N}_F = 1.3 \pm 0.1$ [19] or $\mathcal{N}_F = 1.24 \pm 0.08$ [20], the latter of which LHCb uses [22]. In either case, the biggest limitation is from the form-factor ratio $\mathcal{N}_F$.

A relation between f_s/f_d and $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-) / \text{BR}(\bar{B}^0 \rightarrow D^+ \pi^-)$ is derived along similar lines in [20]. In that case, the form-factor ratio becomes $[f_0^{(s)}(M_\pi^2) / f_0^{(d)}(M_\pi^2)]^2$, i.e., with both numerator and denominator evaluated at $q^2 = M_\pi^2$.

In this paper, we calculate these two form-factor ratios using lattice QCD with $2 + 1$ flavors of sea-quarks. We use the same set of MILC ensembles of gauge configurations [24] and the same sequence of bootstrap copies for both of the B_s^0 and B^0 processes, which reduces the statistical error by correctly accounting for correlations. We include the contributions of the first radially excited states in the fits of correlation functions to avoid the respective systematic errors. Such a treatment turns out to be necessary for calculations at nonzero recoil. By fitting the correlation functions in a simultaneous and mutually constrained manner, we are able to extract the form factors at small recoil. We then extrapolate our lattice results to the continuum limit and to physical quark masses with the guide of chiral perturbation theory. Finally, we use the model-independent z parametrization [25] to extend the form factors toward large recoil.

We finally arrive at the result

$$\frac{f_0^{(s)}(M_\pi^2)}{f_0^{(d)}(M_K^2)} = 1.046(44)(15), \quad (1.6)$$

where the first error is statistical and the second reflects the systematic errors added in quadrature. (Because of refinements in the analysis, Eq. (1.6) differs slightly from our preliminary result [26].) We do not observe a large U -spin breaking effect. Such a small difference between the B_s^0 and B^0 form factors is in accord, however, with recent lattice QCD calculations on lighter mesons like $D_{(s)} \rightarrow \pi(K) \ell \nu$ [27]. It is also in agreement with a result from heavy-meson chiral perturbation theory [28].

The factorization analysis of $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-)/\text{BR}(\bar{B}^0 \rightarrow D^+ \pi^-)$ is somewhat more complicated because of additional topologies in the decay $\bar{B}^0 \rightarrow D^+ \pi^-$. A similar form-factor ratio is needed and, simply by adjusting q^2 in the denominator, we find

$$\frac{f_0^{(s)}(M_\pi^2)}{f_0^{(d)}(M_\pi^2)} = 1.054(47)(17). \quad (1.7)$$

We discuss the implications of our results (1.6) and (1.7) in Sec. VII. Here we only note that both yield fragmentation-fraction ratios f_s/f_d in agreement with LHCb's recent measurement via semileptonic methods [18].

This paper is organized as follows. In Sec. II, we summarize the formalism and our strategy to extract the form factors at nonzero recoil. We provide simulation details in Sec. III. We describe the methodology used to extract the form factors from the two- and three-point correlation functions with the given gauge configurations. This fitting procedure is crucial to our analysis. In Sec. IV we describe the chiral-continuum extrapolation using the corresponding chiral perturbation theory. In Sec. V, these results are then extrapolated to the region of small momentum transfer using a model-independent parametrization. We also compare here a related form factor, which we obtain as a by-product, with the experimental results. In Sec. VI, we account for the systematic errors that arise in our analysis and present a full error budget. Finally, in Sec. VII, we present our results, compare with previous results and discuss prospects and connections to current and future experiments. The Appendix specifies the functional form of the chiral extrapolation in detail.

II. SEMILEPTONIC $B_{(s)} \rightarrow D_{(s)} \ell \nu$ FORM FACTORS FROM LATTICE-QCD

The hadronic matrix elements of the semileptonic decays $B_{(s)} \rightarrow D_{(s)} \ell \nu$ can be parametrized by

$$\begin{aligned} \langle D(p') | \mathcal{V}^\mu | B(p) \rangle = & f_+(q^2) \left[(p + p')^\mu - \frac{M_B^2 - M_D^2}{q^2} q^\mu \right] \\ & + f_0(q^2) \frac{M_B^2 - M_D^2}{q^2} q^\mu, \end{aligned} \quad (2.1)$$

where $q = p - p'$ is the momentum transfer and $\mathcal{V}^\mu = \bar{c} \gamma^\mu b$ is the (continuum) vector current. Another parametrization uses velocity 4-vectors $v = p/M$ instead of momentum p [29],

$$\frac{\langle D(p') | \mathcal{V}^\mu | B(p) \rangle}{\sqrt{M_B M_D}} = h_+(w)(v + v')^\mu + h_-(w)(v - v')^\mu, \quad (2.2)$$

where $w = v \cdot v' = (M_B^2 + M_D^2 - q^2)/2M_B M_D$ describes the recoil of the process. The $h_\pm$ parametrization is convenient for lattice QCD, both for numerical simulation [30] and for matching lattice gauge theory to continuum QCD [31,32].

The lattice QCD calculation of h_+ in the zero-recoil limit has been investigated using double ratios [30],

$$R_+ = \frac{\langle D | \bar{c} \gamma^0 b | B \rangle \langle B | \bar{b} \gamma^0 c | D \rangle}{\langle D | \bar{c} \gamma^0 c | D \rangle \langle B | \bar{b} \gamma^0 b | B \rangle} = |h_+(1)|^2 \quad (2.3)$$

with all states at rest. To proceed analogously at nonzero momentum, we introduce the following single ratios:

$$\mathbf{a} \equiv \frac{\langle D(p) | \bar{c} \gamma b | B(\mathbf{0}) \rangle}{\langle D(\mathbf{0}) | \bar{c} \gamma^0 b | B(\mathbf{0}) \rangle} = \frac{h_+(w) - h_-(w)}{2h_+(1)} \mathbf{v}, \quad (2.4)$$

$$\mathbf{b} \equiv \frac{\langle D(p) | \bar{c} \gamma b | B(\mathbf{0}) \rangle}{\langle D(p) | \bar{c} \gamma^0 b | B(\mathbf{0}) \rangle} = \frac{h_+(w) - h_-(w)}{(w+1)h_+(w) - (w-1)h_-(w)} \mathbf{v}, \quad (2.5)$$

$$\mathbf{d} \equiv \frac{\langle D(p) | \bar{c} \gamma c | D(\mathbf{0}) \rangle}{\langle D(p) | \bar{c} \gamma^0 c | D(\mathbf{0}) \rangle} = \frac{\mathbf{v}}{1+w}, \quad (2.6)$$

where the last follows from vector current conservation, $h^{D \rightarrow D}(w) = 0$.

We can write down the equations that manifest the relations between the ratios and the form factors

$$w = \frac{1 + \mathbf{d} \cdot \mathbf{d}}{1 - \mathbf{d} \cdot \mathbf{d}}, \quad (2.7)$$

$$\frac{h_+(w)}{h_+(1)} = \frac{a_i}{b_i} - \mathbf{a} \cdot \mathbf{d}, \quad (2.8)$$

$$\frac{h_-(w)}{h_+(1)} = \frac{a_i}{b_i} - \frac{a_i}{d_i}. \quad (2.9)$$

In Eq. (2.4), we have a ratio $\mathbf{a}$ between matrix elements involving a final D meson with nonzero and zero spatial momentum. The purpose is to make use of the correlations in the uncertainties between the two. The form factor at zero recoil can be extracted precisely via R_+ [30], and we find that these ratios aid calculations at nonzero recoil in a similar way.

With $h_\pm(w)$ in hand, one can obtain the form factors $f_+(q^2)$ and $f_0(q^2)$,

$$f_+(q^2) = \frac{1}{2\sqrt{r}} [(1+r)h_+(w) - (1-r)h_-(w)], \quad (2.10)$$

$$f_0(q^2) = \sqrt{r} \left[\frac{w+1}{1+r} h_+(w) - \frac{w-1}{1-r} h_-(w) \right], \quad (2.11)$$

where $r = M_D/M_B$ and $q^2 = M_B^2 + M_D^2 - 2wM_B M_D$. Equations (2.8) and (2.9) both contain the factor $h_+(1)$, so we write

$$f_0(q^2) = h_+(1) \tilde{f}_0(w(q^2)). \quad (2.12)$$

In the formulas until now, we have not specified the spectator mass, so they apply to both the $B \rightarrow D$ and $B_s \rightarrow D_s$ processes. With this notation, the desired ratio of the form factors is then

$$\frac{f_0^{B_s \rightarrow D_s}(M_\pi^2)}{f_0^{B \rightarrow D}(M_K^2)} = \frac{h_+^{B_s \rightarrow D_s}(1) \tilde{f}_0^{B_s \rightarrow D_s}(w(M_\pi^2))}{h_+^{B \rightarrow D}(1) \tilde{f}_0^{B \rightarrow D}(w(M_K^2))}, \quad (2.13)$$

where the first factor is obtained from the ratios $R_+^{B \rightarrow D}$ and $R_+^{B_s \rightarrow D_s}$ and the last from the expressions in Eqs. (2.8) and (2.9).

On the lattice, we define a vector current $V^\mu = Z_{V_{cc}}^{1/2} Z_{V_{bb}}^{1/2} \bar{\Psi}_c \gamma^\mu \Psi_b$ [30,32], where the factors $Z_{V_{cc}}^{1/2}$ normalize the flavor charge. The matching between the lattice and the continuum physics can be bridged by the relation $\mathcal{V}^\mu = \rho_{V^\mu} V^\mu$, where $\rho_{V^\mu}^2 = Z_{V_{bc}}^4 Z_{V_{cb}}^4 / Z_{V_{bb}}^4 Z_{V_{cc}}^4$. The normalization factors $Z_{V_{cc}}^{1/2}$ cancel in the ratios in Eqs. (2.3), (2.4), (2.5), and (2.6). The factor ρ_{V^μ} has been verified to be very close to 1 with one-loop perturbation theory with unimproved gluons [32]. Calculations of ρ_{V^μ} with improved gluons (as used here; cf. Sec. III) are in progress. Given the ratio structure in Eq. (2.13), it is clear that the (small) contributions from $\rho_{V^\mu} - 1$ should largely cancel. Thus, in this analysis, we take $\rho_{V^\mu} = 1$ and estimate the uncertainty from this choice in Sec. VI.

III. SIMULATIONS AND FITTING METHODOLOGY

A. Data setup and the lattice simulations

Our calculation uses four ensembles of MILC's (2 + 1)-flavor asqtad configurations [24] at two lattice spacings, $a \approx 0.12$ fm, 0.09 fm, which we refer to as the “coarse” and “fine” lattices, respectively. The configurations were generated with an $O(a^2)$ Symanzik improved gauge action [33–36]. The coarse (fine) ensembles used here have a lattice size of $20^3 \times 64$ ($28^3 \times 96$), so in both cases the spatial size is $L \approx 2.4$ fm. The four ensembles have different sea-quark masses, so, for the sake of convenience, we label them C020, C007, F0062, and F0124. Details on the parameters that we use in the simulations are summarized in Table I. The strange and light sea-quarks are simulated using the asqtad-improved staggered action [37–41]. The asqtad action is also used for our strange and light valence quarks. The heavy charm and bottom quarks are simulated using the Sheikholeslami-Wohlert clover action [42] with the Fermilab interpretation [43]. We simulate the $B \rightarrow D$ and $B_s \rightarrow D_s$ decays on the same ensembles, so that correlations reduce the statistical uncertainty in the ratios. For the $B \rightarrow D$ decay, the valence

light-quark mass is taken to be the same as the sea-quark mass, i.e., we stick to “full QCD” data with $m_x = m_l$, while for the $B_s \rightarrow D_s$ process, we set the valence strange-quark mass to be close to its physical value, $m_x = m_s$. The charm and bottom quarks in our calculation are tuned to their physical values up to a tuning uncertainty. Columns 2–9 in Table I list, respectively, the approximate lattice spacings, light/strange sea-quark masses, number of configurations, the hopping parameter $\kappa_{b(c)}$, the coefficient for the clover term c_{SW} , and the light valence-quark masses used in the $B \rightarrow D$ and $B_s \rightarrow D_s$ simulations. The quark masses here are all in lattice units.

We obtain the matrix elements appearing in Sec. II from the following three-point correlation functions:

$$C_3^{DV^B}(0, t, T; \mathbf{p}) = \sum_{\mathbf{x}, \mathbf{y}} \langle \mathcal{O}_D(0, \mathbf{0}) \bar{\Psi}_c i \gamma^\mu \Psi_b(t, \mathbf{y}) \mathcal{O}_B^\dagger(T, \mathbf{x}) \rangle e^{i\mathbf{p} \cdot \mathbf{y}}, \quad (3.1)$$

$$C_3^{DV^D}(0, t, T; \mathbf{p}) = \sum_{\mathbf{x}, \mathbf{y}} \langle \mathcal{O}_D(0, \mathbf{0}) \bar{\Psi}_c i \gamma^\mu \Psi_c(t, \mathbf{y}) \mathcal{O}_D^\dagger(T, \mathbf{x}) \rangle e^{i\mathbf{p} \cdot \mathbf{y}}, \quad (3.2)$$

$$C_3^{BV^B}(0, t, T; \mathbf{0}) = \sum_{\mathbf{x}, \mathbf{y}} \langle \mathcal{O}_B(0, \mathbf{0}) \bar{\Psi}_b i \gamma^4 \Psi_b(t, \mathbf{y}) \mathcal{O}_B^\dagger(T, \mathbf{x}) \rangle, \quad (3.3)$$

where the sum over $\mathbf{x}$ sets the B meson at rest, and the sum over $\mathbf{y}$ selects the final-state D -meson momentum. The final D meson is simulated with several small spatial momenta which are the lowest possible values for the finite spatial volumes: $\mathbf{p} = 2\pi(0, 0, 0)/L$, $2\pi(1, 0, 0)/L$, $2\pi(1, 1, 0)/L$, $2\pi(1, 1, 1)/L$, $2\pi(2, 0, 0)/L$, and permutations. To increase statistics, data are generated at four different source times, spaced evenly along the temporal extent of the lattice. The zero-momentum correlation functions for $D \rightarrow D$ and $B \rightarrow B$ serve as normalization, as discussed above. The $D \rightarrow D$ correlation-function with a nonzero final-state momentum is used to extract w via Eqs. (2.6) and (2.7).

The analysis below also requires the two-point function

$$C_2^X(t, \mathbf{p}) = \sum_{\mathbf{x}} e^{i\mathbf{p} \cdot \mathbf{x}} \langle \mathcal{O}_X^\dagger(t, \mathbf{x}) \mathcal{O}_X(0, \mathbf{0}) \rangle, \quad (3.4)$$

where $X = B$ or D .

We simulate the daughter meson with two different choices for the interpolation operator $\mathcal{O}_X$: with a 1S-wave

TABLE I. Parameters of the MILC asqtad ensembles of configurations and the valence quarks used in this analysis.

Ensemble	a (fm)	am_l/am_h	N_{confs}	κ_c	κ_b	c_{SW}	$am_x(B \rightarrow D)$	$am_x(B_s \rightarrow D_s)$
C020	≈ 0.12	0.020/0.050	2052	0.1259	0.0918	1.525	0.020	0.0349
C007	≈ 0.12	0.007/0.050	2110	0.1254	0.0901	1.530	0.007	0.0349
F0124	≈ 0.09	0.00124/0.031	1996	0.1277	0.0982	1.473	0.0124	0.0261
F0062	≈ 0.09	0.0062/0.031	1931	0.1276	0.0979	1.476	0.0062	0.0261

smearing and without any smearing [44]. The smearing optimizes the overlap of the operator with the ground-state wave function of the meson, so the two choices have different excited-state contributions but the same energies. For the three-point correlation functions, we always use a 1S-smearing source for the extended quark propagator.

B. From correlators to form factors

In general, two- and three-point functions, such as those in Eqs. (3.1), (3.2), (3.3), and (3.4), can be expressed as [45],

$$C_2^X(t, \mathbf{p}) = \sum_{k=0} (-1)^{kt} |Z_k(\mathbf{p})|^2 [e^{-E_k(\mathbf{p})t} + e^{-E_k(\mathbf{p})(T-t)}], \quad (3.5)$$

$$C_3^{YV^\mu X}(0, t, T; \mathbf{p}) = \sum_k \sum_\ell (-1)^{kt} (-1)^{\ell(T-t)} A_{k\ell}^\mu(\mathbf{p}) \times e^{-E_k(\mathbf{p})t} e^{-M_\ell(T-t)} \quad (3.6)$$

where $E_k(M_\ell)$ are the energy levels of $Y(X)$ and $A_{k\ell}^\mu$ are coefficients of the transition $X_\ell \rightarrow Y_k$. We use four states to fit the two-point functions in Eq. (3.5). We include the same set of states to fit the three-point functions and the number of states can be reduced to two (the ground and first excited states) by using some averaging method (next paragraph). If the time differences between the source (0) and vector current (t) and that between vector current and sink (T) in Eq. (3.6) are sufficiently large, i.e., $|t| \rightarrow \infty$ and $|T - t| \rightarrow \infty$, only the lowest energy level will survive. Then, we have ($B_s \rightarrow D_s$ follows similarly)

$$R_+ \leftarrow \frac{C_3^{DV^4B}(0, t, T; \mathbf{0})}{C_3^{BV^4B}(0, t, T; \mathbf{0})} \frac{C_3^{BV^4D}(0, t, T; \mathbf{0})}{C_3^{DV^4D}(0, t, T; \mathbf{0})}, \quad (3.7)$$

$$a_i \leftarrow \frac{C_3^{DV^iB}(0, t, T; \mathbf{p})}{C_3^{DV^4B}(0, t, T; \mathbf{0})} \left(\frac{|Z_0(\mathbf{0})|}{|Z_0(\mathbf{p})|} \sqrt{\frac{E_0(\mathbf{p})}{E_0(\mathbf{0})}} e^{[E_0(\mathbf{p}) - E_0(\mathbf{0})]t} \right), \quad (3.8)$$

$$b_i \leftarrow \frac{C_3^{DV^iB}(0, t, T; \mathbf{p})}{C_3^{DV^4B}(0, t, T; \mathbf{p})}, \quad (3.9)$$

$$d_i \leftarrow \frac{C_3^{DV^iD}(0, t, T; \mathbf{p})}{C_3^{DV^4D}(0, t, T; \mathbf{p})}, \quad (3.10)$$

where $\leftarrow$ means that the left-hand side is output of an analysis procedure. In practice, the separations between the current insertion and the source/sink, t and $T - t$, are often not large enough to suppress the excited states completely. The factor inside the parentheses in Eq. (3.8) cancels the leading time dependence of the ratio of three-point functions with different momenta; both $Z_0(\mathbf{p})$ and $E_0(\mathbf{p})$ come from fitting C_2^D as suggested by Eq. (3.5). Instead of fitting for plateaus, we extract the matrix-element ratios on the left-hand sides of Eqs. (3.7), (3.8), (3.9), and (3.10) by fitting the right-hand sides in a way that incorporates excited states.

We can write the first few terms in Eq. (3.6) as [44]

$$C_3^{YV^\mu X}(0, t, T) = A_{00}^\mu(t) + (-1)^t A_{10}^\mu(t) + (-1)^{T-t} A_{01}^\mu(t) + (-1)^T A_{11}^\mu(t) + A_{02}^\mu(t) + A_{20}^\mu(t) + \text{higher excitations}, \quad (3.11)$$

where $A_{k\ell}^\mu(t) \equiv A_{k\ell}^\mu e^{-E_k t} e^{-M_\ell(T-t)}$. The terms A_{10} , A_{01} , A_{11} are the contributions from the opposite-parity states that are introduced by the operator involving staggered quarks. We can reduce their effects by making use of the fact that they oscillate with either t or T . The contamination from A_{10} and A_{01} is minor because no obvious oscillation is visible with any of the three-point functions. Based on the plots of the ratios calculated from different source-sink separations T , there is no sizable contribution from A_{11} either. With the four source times, which are evenly distributed in the temporal interval of the lattice, we separate two of the sinks from the sources by an even number of time slices and the other two by a neighboring odd number. We apply the following averaging method to further reduce the effect from A_{11} [44]

$$\bar{R}(0, t, T) = \frac{1}{2}R(0, t, T) + \frac{1}{4}R(0, t, T+1) + \frac{1}{4}R(0, t+1, T+1) \quad (3.12)$$

where R stands for any of the correlation-function ratios corresponding to R_+ , a_i , b_i , or d_i . With this averaging procedure, the A_{11} terms are suppressed by a factor of 6–10 and the A_{01} and A_{10} terms, already small, are suppressed by a factor of about 2. Hence, the systematic error arising from neglecting terms A_{01} , A_{10} , and A_{11} can be safely dropped.

The foregoing analysis enables us to use a simple fitting scheme for the ratios including only the contributions from A_{00} , A_{20} , A_{02} . At the lowest order, the functional forms for determining a_i , b_i , and d_i are then

$$\begin{aligned} & \frac{C_3^{DV^iB}(0, t, T; \mathbf{p})}{C_3^{DV^4B}(0, t, T; \mathbf{0})} \frac{|Z_0(\mathbf{0})|}{|Z_0(\mathbf{p})|} \sqrt{\frac{E_0(\mathbf{p})}{E_0(\mathbf{0})}} e^{[E_0(\mathbf{p}) - E_0(\mathbf{0})]t} \\ &= a_i [1 + \mathcal{A}_{02} e^{-\Delta M(T-t)} + \mathcal{A}_{20} e^{-\Delta E(\mathbf{p})t} \\ & \quad + \mathcal{A}'_{20} e^{-\Delta E(0)t}] e^{\delta t}, \end{aligned} \quad (3.13)$$

$$\frac{C_3^{DV^iB}(0, t, T; \mathbf{p})}{C_3^{DV^4B}(0, t, T; \mathbf{p})} = b_i [1 + \mathcal{B}_{02} e^{-\Delta M(T-t)} + \mathcal{B}_{20} e^{-\Delta E(\mathbf{p})t}], \quad (3.14)$$

$$\frac{C_3^{DV^iD}(0, t, T; \mathbf{p})}{C_3^{DV^4D}(0, t, T; \mathbf{p})} = d_i [1 + \mathcal{D}_{02} e^{-\Delta E(0)(T-t)} + \mathcal{D}_{20} e^{-\Delta E(\mathbf{p})t}]. \quad (3.15)$$

The fit parameter δ in Eq. (3.13) allows for imperfect cancellation of the leading t dependence. The parameters $\Delta E(\mathbf{p}) = E_2(\mathbf{p}) - E_0(\mathbf{p})$ ($\Delta M = M_2 - M_0$) denote the splittings between the D -meson energy (B -meson mass)

and its first radial excitation. We find that the double ratio R_+ is so weakly affected by excited states that it suffices to fit it to a constant in t . Adding terms to describe excited states in R_+ leads to changes no bigger than the statistical errors. The energy splittings $\Delta E(\mathbf{p})$, ΔM in these expressions are also constrained by the two-point functions, Eq. (3.5).

We employ two fit procedures to determine the ratios. One, which we explain first, is simpler. The other is more complicated but yields better results, as we explain below, so we take it as our primary analysis and use the simple method as a cross check.

C. Two-step fit

The simpler method proceeds in two steps. We first fit the two-point functions to obtain the energies, energy splittings, and overlaps: $E(\mathbf{p})$, $\Delta E(\mathbf{p})$, ΔM , and $Z(\mathbf{p})$. We use constrained curve fitting and priors [46,47]. The priors in these fits impose no real constraint. Second, we take the

energy splittings from these two-point fits as priors when fitting the ratios of three-point functions. The priors for the amplitudes on the right-hand sides of Eqs. (3.13), (3.14), and (3.15) are again taken wide enough to impose no real constraint. Below we call this approach the “two-step fit.”

As discussed above, we have data for smeared and local interpolating operators. These different correlator ratios have different excited-state contributions. To determine the matrix-element ratios, we fit the correlation-function ratios of the two smearing types either separately or simultaneously, as illustrated in Fig. 2. Although the two smearing types follow rather different curves, they arrive at consistent values of a_i , b_i , and d_i as described in Eqs. (3.13), (3.14), and (3.15). Figure 2 shows that the separate fit and the simultaneous fit give consistent results for the ratio d_i . The other two single ratios a_i , b_i can be determined in a similar way, which can be seen in the sample fit in Fig. 3.

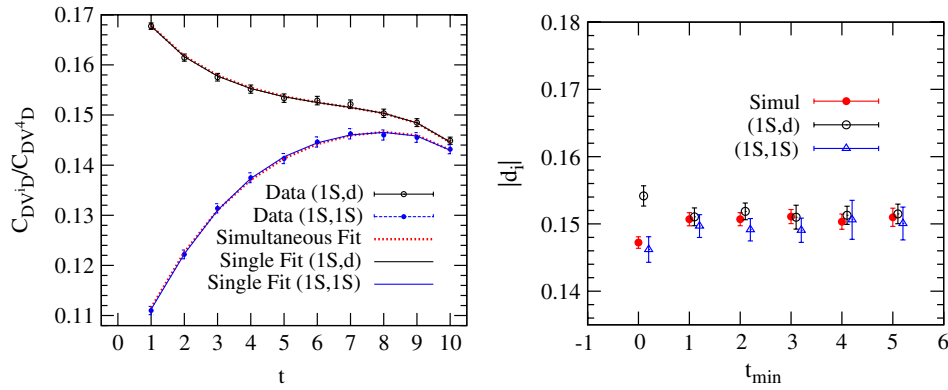


FIG. 2 (color online). A sample fit of the single ratio d_i with the final D meson carrying momentum $\mathbf{p} = 2\pi(1, 0, 0)/L$ on the ensemble C020. The left graph shows the data with 1S-smearing (1S, 1S) (filled circles, data along the bottom curve) and that with partial smearing (1S, d) (open circles, data along the top curve) fitted separately (solid curves) and simultaneously (dashed curves). The (1S, 1S), (1S, d), and simultaneous fits have $\chi^2/\text{d.o.f.} = 1.0, 1.1$ and 0.85 , respectively. Fit results over the interval $t \in [t_{\min}, 10]$ are shown in the right graph and are seen to be stable for $t_{\min} \geq 1$.

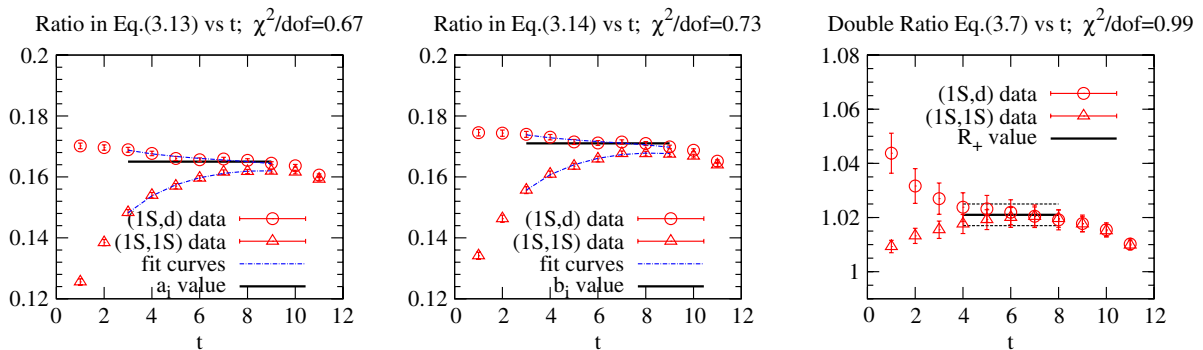


FIG. 3 (color online). Sample fits of the ratios a_i , b_i , and R_+ from the ensemble C020. The triangles and circles correspond to the data with 1S smearing (1S, 1S) and partial smearing (1S,d), respectively. In the first two graphs, the final D meson carries a spatial momentum $\mathbf{p} = 2\pi(1, 0, 0)/L$. The dot-dashed curves indicate the best fits and they are in good agreement with the data points. The third graph shows the fit for the double ratio R_+ . The horizontal lines in these graphs show the resulting values of a_i , b_i , and R_+ , as well as the ranges included in the fits.

D. Combined fit

Our preferred fit treats the two-point functions and three-point-function ratios simultaneously. This approach allows all correlation functions to influence the output energies and overlaps, combining all information at hand, including the correlations between the two- and various three-point functions. We refer to this procedure as our “combined fit,” in contrast with the two-step fit described above. In particular, all correlation functions are then treated on the same footing in the determination of the energy splittings. Figure 4 shows the relationships between the ratios and two-point functions, building up constraints among correlation functions of zero and nonzero final momenta. The single ratios a_i also require the two-point $Z(\mathbf{p})$ factors from the relevant three two-point functions.

The combined fit is repeated for each value of the momentum. The resulting single ratios a_i , b_i , and d_i and the double ratio R_+ at the corresponding recoil are then used to compute the form-factor ratios $h_{\pm}(w)/h_{\pm}(1)$ and

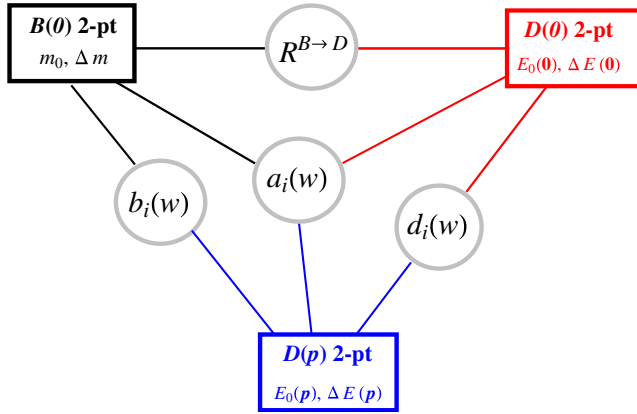


FIG. 4 (color online). Diagram showing which correlators and correlator ratios influence energies and amplitude ratios. Energy splittings of the initial and final mesons $B(0)$, $D(0)$, and $D(p)$ are determined from the two-point functions (boxes) as well as the ratios (circles). The lines connecting them indicate their common dependence on the splittings. Altogether seven correlation functions are included in the combined fit.

$h_+(1)$. To verify the results from the two approaches, we compare the resulting $h_+(w)$ of the two coarse ensembles C007, C020 in Fig. 5. In general, they are in very good agreement at the five values of w where we have data, while the combined fit has slightly better precision at small recoil.

The combined fit turns out to have other more important advantages over the two-step fit. First, the resulting $h_{\pm}(w)/h_{\pm}(1)$ is more stable with the combined fit than the two-step fit, where the fitting range must be determined carefully. This stability stems from the fact that the combined fit does a better job of resolving the correlated statistical fluctuations at zero and nonzero recoil. Second, the combined fit helps to reduce the systematic error due to excited states. We account for the excited-state contribution in the fit for single ratios to work around the fact that sink-source separations cannot be taken satisfactorily large. Although the towers of the excited states are not the focus of this paper, the proper accounting of their contributions is important, because they influence ratio results. The combined fit procedure resolves the excited states more stably than the two-step fit. Third, the resulting form factors $h_{\pm}(w)$ using the combined fit at these values of w are more consistent with each other than those using the two-step fit. This can be seen when one attempts to fit the results at different recoil to a chiral effective theory. Section IV shows that the combined fit procedure results in a more reliable chiral extrapolation than the two-step fit, and hence we use it throughout our analysis. That said, as shown in Fig. 5 and Table II, the two fitting procedures give seemingly good pointwise consistency.

Although the combined fit method helps in many aspects, it requires the handling of a larger data set and correspondingly a much larger covariance matrix. We use the jackknife method with single elimination to calculate the covariance matrices because the data samples show a very small autocorrelation time (less than 1). To reduce the time searching for the minimum of χ^2 , we take the output of the two-step fit as the initial guess for the combined fit.

It is worth mentioning a small complication. When fitting the single ratio a_i , we need in advance both the

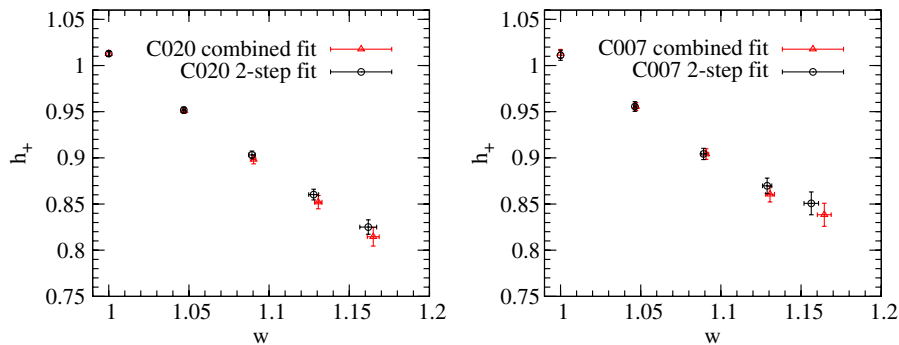


FIG. 5 (color online). Comparison of $h_+(w)$ obtained from the two-step fit and combined fit for the two coarse ensembles C020 (left) and C007 (right).

TABLE II. Comparison of the results of w [from Eq. (2.7)] and h_+ [from Eqs. (2.3) and (2.8)] using 2-step fit and combined fit procedures.

momentum ($2\pi/L$)		C007 (2-step)	C007 (combined)	C020 (2-step)	C020 (combined)
(0,0,0)	w	1	1	1	1
	h_+	1.011(6)	1.013(4)	1.013(3)	1.013(2)
(1,0,0)	w	1.0464(9)	1.0470(7)	1.0468(10)	1.0470(6)
	h_+	0.956(5)	0.956(4)	0.952(3)	0.951 (3)
(1,1,0)	w	1.089(2)	1.091(2)	1.089(2)	1.090(1)
	h_+	0.904(6)	0.904(4)	0.903(4)	0.898(5)
(1,1,1)	w	1.129(3)	1.131(3)	1.128(3)	1.131(2)
	h_+	0.870(8)	0.861(6)	0.860(6)	0.852(7)
(2,0,0)	w	1.156(5)	1.164(4)	1.162(5)	1.165(4)
	h_+	0.851(12)	0.838(12)	0.825(8)	0.815(10)

ground-state energy E_0 and the wave function normalization factor Z to suppress the time dependence of the ratio. With the combined fit procedure, E_0 and Z are refined through the two-point functions which are part of the combined fitting. So in the actual analysis, we take the results of E_0 and Z from the combined fit and plug them back to suppress the time dependence of the three-point function for a_i . We need to iterate such a process a few times until the fitting results stabilize. We find that this iteration converges within two or three steps.

IV. CHIRAL-CONTINUUM EXTRAPOLATION

Given the light-quark masses in Table I, we extrapolate the results to the physical value guided by chiral effective theory. In the case of $h_+(w)$, we follow rooted staggered chiral perturbation theory (rS χ PT) [48–52]. The specific application to the case of $B \rightarrow D^{(*)}$ at zero recoil is provided in Refs. [44,53]. The continuum χ PT for the semileptonic $B \rightarrow D^{(*)}$ form factor at nonzero recoil has been derived at next-to-leading order (NLO) in Ref. [54], and the generalization to rS χ PT for $B \rightarrow D$ is given in the Appendix. In the case of $h_-(w)$, the leading correction is simply a constant that is inversely proportional to the charm quark mass. To describe the simulated data, we also must parametrize the recoil dependence to quadratic order around zero recoil. The expansion coefficients are related to the slope and curvature of the form factors.

Thus, we can write the general expression for $h_{\pm}(w)$ with NLO rS χ PT and higher-order analytic terms incorporating lattice spacing dependence as

$$\begin{aligned}
 h_+^{\text{lat}}(w) = & 1 - \rho_+^2(w-1) + k_+(w-1)^2 + \frac{X_+(\Lambda_\chi)}{m_c^2} \\
 & + \frac{g_{D^*D\pi}^2}{16\pi^2 f^2} \log_{\text{S1-loop}}(\Lambda_\chi, w) + c_{0,+}m_x \\
 & + c_{1,+}(2m_l + m_h) + c_{a,+}a^2,
 \end{aligned} \tag{4.1}$$

$$\begin{aligned}
 h_-^{\text{lat}}(w) = & \frac{X_-}{m_c} - \rho_-^2(w-1) + k_-(w-1)^2 + c_{0,-}m_x \\
 & + c_{1,-}(2m_l + m_h) + c_{a,-}a^2,
 \end{aligned} \tag{4.2}$$

where $-\rho_{\pm}^2$ and $2k_{\pm}$ are the slopes and curvatures of the form factors, while $X_{\pm}$ are low-energy constants. In the case of $h_+(w)$, X_+ depends on the chiral scale Λ_χ in such a way as to cancel the Λ_χ dependence of the nonanalytic terms (“chiral logs”). These terms, denoted here as $\log_{\text{S1-loop}}$, are given by the terms appearing inside the square brackets in Eqs. (A2) and (A3) of the Appendix. The other form factor $h_-(w)$ has no nonanalyticity at one-loop. Equations (4.1) and (4.2) also include terms depending linearly on the valence (m_x) and sea (m_l and m_s) quark masses, with coefficients $c_{0(1),\pm}$. These terms are next-to-next-to-leading order (NNLO) in the chiral expansion and are needed to describe the data with m_x or $m_l \gtrsim \frac{1}{2}m_s$. Generic lattice spacing dependence is described by the terms with coefficients $c_{a,\pm}$.

We treat the chiral extrapolations of the $B \rightarrow D$ and $B_s \rightarrow D_s$ data slightly differently. For $B \rightarrow D$, we analyze only full QCD data points, i.e., $m_x = m_l$. Then, since the strange sea-quark in all ensembles is tuned within several per cent of its physical mass, $m_h \approx m_s$, the dependence of the form factors on the sea- and valence-quark masses cannot be disentangled. Therefore, we drop the parameter $c_{1,+}$ when fitting the $B \rightarrow D$ data. For our $B_s \rightarrow D_s$ data, on the other hand, the strange valence-quark is tuned close to its physical mass for all the ensembles we analyze, $m_x = m_s$. As a result, we cannot disentangle the valence-quark dependence. Therefore, we discard the parameter $c_{0,\pm}$ when fitting the $B_s \rightarrow D_s$ data, and estimate the tuning error of m_s *a posteriori* in Sec. VID.

The rS χ PT expression for $\log_{\text{S1-loop}}(\Lambda_\chi, w)$ contains several low-energy constants used in rS χ PT to describe the masses and decay constant of light pseudoscalar mesons. The values we use for these parameters are taken from Refs. [24,55] and given in Table III. The χ PT expressions also require the $D_{(s)} - D_{(s)}^*$ splitting $\Delta^{(c)}$ and the

TABLE III. Input parameters for the chiral extrapolation [24,55].

rs χ PT quantity	Ensemble			
	C020	C007	F0062	F0124
r_1/a	2.821123	2.738591	3.857729	3.788732
μ_0	6.234000	6.234000	6.381592	6.381592
$r_1^2 a^2 \Delta_P$	0	0	0	0
$r_1^2 a^2 \Delta_A$	0.2052872	0.2052872	0.0706188	0.0706188
$r_1^2 a^2 \Delta_T$	0.3268607	0.3268607	0.1153820	0.1153820
$r_1^2 a^2 \Delta_V$	0.4391099	0.4391099	0.1523710	0.1523710
$r_1^2 a^2 \Delta_I$	0.5369975	0.5369975	0.2062070	0.2062070
$r_1^2 a^2 \delta'_V$	-0.05	-0.05	-0.03	-0.03
$r_1^2 a^2 \delta'_A$	-0.28	-0.30	-0.15	-0.16

TABLE IV. Chiral extrapolation of the two-step and combined fit results on the coarse ensembles.

Form factor	Two-step fit		Combined fit	
	$\chi^2/\text{d.o.f.}$	p value	$\chi^2/\text{d.o.f.}$	p value
$h_+^{B \rightarrow D}(w)$	11/7	0.14	3.7/7	0.81
$h_+^{B_s \rightarrow D_s}(w)$	11/7	0.13	5/7	0.68

pion decay constant f_π ; we take both from Ref. [17]. To combine data from both lattice spacings, we convert dimensionful quantities to r_1 units, where r_1 is the distance defined via the interquark force by $r_1^2 F(r_1) = 1$ [56,57]. We take r_1/a from Refs. [24,55].

Unfortunately, the $D^* - D - \pi$ coupling $g_{D^* D \pi}$ and similar couplings with strange mesons, which appear in the coefficient $g_{D^* D \pi}^2/16\pi^2 f_\pi^2$ of the chiral log terms, are not known with good precision. We appeal to various estimates of $g_{D^* D \pi}$ available in the literature, including CLEO's measurement of the D^* width: $g_{D^* D \pi} = 0.59(7)$ [58]; quenched lattice QCD: $g_{D^* D \pi} = 0.67(8)(^{+4}_{-6})$ [59]; a fit to various experimental data, including the D^* width: $g_{D^* D \pi} = 0.51$ (no error reported) [60]; two-flavor lattice QCD in the static limit: $g_{D^* D \pi} = 0.516(51)$ [61]; and

2 + 1-flavor lattice QCD in the static limit: $g_{D^* D \pi} = 0.449(51)$ [62]. In this calculation, we include $g_{D^* D \pi}$ as a parameter in the constrained fit with a prior 0.51 ± 0.20 .

In Sec. III, we compared the two fitting procedures, two-step fit and combined fit, with which we obtain the single ratios a_i , b_i , d_i , and the double ratio R_+ . At each w where we have data, $h_+(w)$ from the two procedures are in good agreement (within 1σ). We then fit the resulting $h_+(w)$ for the coarse ensembles (C020 and C007) to Eq. (4.1) without the analytic terms and the a^2 dependence (NLO). The results are shown in Table IV. It is apparent that the results from the combined fit procedure are better described by the chiral effective theory that we employ, giving a $\chi^2/\text{d.o.f.} = 0.53$ for $B \rightarrow D$ (compared to 1.6 from the two-step fit). A similar observation can be found in the case of $B_s \rightarrow D_s$. This indicates that the correlations among the ratios and those among different kinematic points are better resolved by the combined fit, and hence we follow this procedure for the entire analysis.

The results of the chiral-continuum extrapolation of $h_+(w)$ for $B \rightarrow D$ and $B_s \rightarrow D_s$ are plotted in Fig. 6. With the large number of configurations we have for the four ensembles, we are able to determine the form factors $h_+(w)$ with statistical errors at the level of $\sim 0.5\%$ at zero recoil, increasing to $\sim 1.5\%$ at $w = 1.15$. The form factor $h_+(w)$ for both of the $B \rightarrow D$ and $B_s \rightarrow D_s$ decays exhibits a small dependence on the light-quark masses and lattice spacings, so the extrapolated physical values are close to the lattice data. The difference between $h_+^{B \rightarrow D}(w)$ and $h_+^{B_s \rightarrow D_s}(w)$ is also small. The form factor with strange spectator $h_+^{B_s \rightarrow D_s}(w)$ shows a steeper slope and larger curvature— $\rho_+^2 = 1.26(09)$ and $k_+ = 1.15(9)$ —than its $B \rightarrow D$ counterpart— $\rho_+^2 = 1.14(10)$ and $k_+ = 0.87(13)$.

The results of the chiral-continuum extrapolation of $h_-(w)$ for $B \rightarrow D$ and $B_s \rightarrow D_s$ are plotted in Fig. 7. Here light-quark mass (both sea and spectator) and lattice spacing dependence are visible. We find an ≈ 0.04 difference between the two values of $h_-(1)$ at zero recoil. From Eq. (2.11), however, this effect does not cause

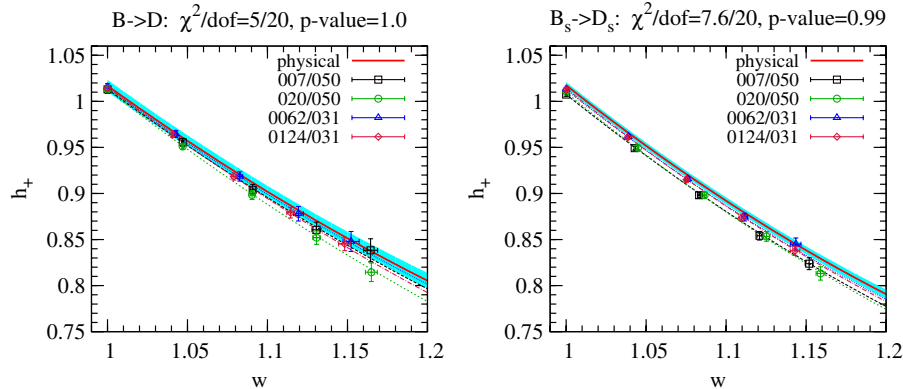


FIG. 6 (color online). Chiral-continuum extrapolation of $h_+(w)$ for $B \rightarrow D$ (left) and $B_s \rightarrow D_s$ (right) decays based on the four ensembles listed in Table I. The blue bands show only the statistical errors and the red curves are the chiral and continuum limits.

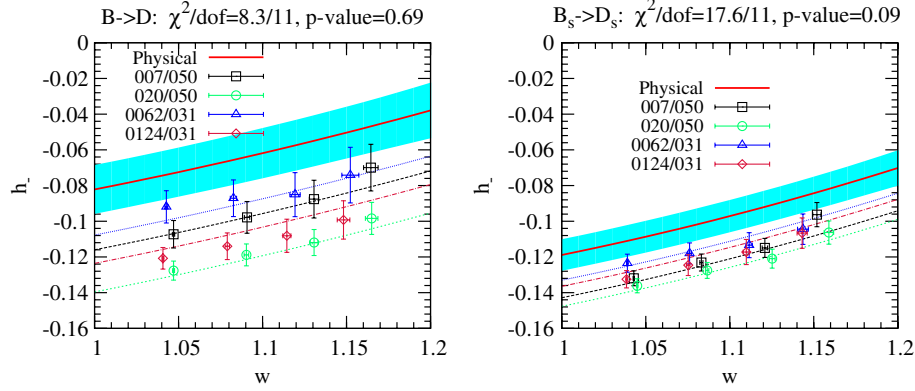


FIG. 7 (color online). Chiral-continuum extrapolation of $h_-(w)$ for $B \rightarrow D$ (left) and $B_s \rightarrow D_s$ (right) decays based on the four ensembles listed in Table I. The blue bands show only the statistical errors and the red curves are the chiral and continuum limits.

much difference in f_0 . We therefore anticipate that the U -spin symmetry breaking effect is smaller than what was found in Ref. [23]. Such an observation is in accord with the recent lattice calculations of f_+ , f_0 in the $D_{(s)} \rightarrow \pi(K)$ decays [27].

With the results from the chiral-continuum extrapolation in hand, we now convert $h_{\pm}(w)$ into $f_+(q^2)$ and $f_0(q^2)$ with Eqs. (2.10) and (2.11) and the physical B and D masses [17]. To gain confidence in our procedures, let us compare the resulting f_+ with experimental measurements. The differential decay rate of $B \rightarrow D$ is given by

$$\frac{d\Gamma(\bar{B}^0 \rightarrow D\ell\bar{\nu})}{dw} = \frac{G_F^2}{48\pi^3} M_D^3 (M_B + M_D)^2 (w^2 - 1)^{3/2} |V_{cb}|^2 \times |\mathcal{G}(w)|^2, \quad (4.3)$$

where G_F is the Fermi constant, and it is conventional to introduce

$$\mathcal{G}(w) = \frac{2\sqrt{r}}{1+r} f_+(w). \quad (4.4)$$

Experiments report the zero-recoil form factor $|V_{cb}|\mathcal{G}(1)$ and the relative form-factor slope $\rho^2 \equiv -\mathcal{G}'(1)/\mathcal{G}(1)$ [63]. From our extrapolated data, we find $\mathcal{G}(1) = 1.058(9)_{\text{stat}}$, which is consistent with the previous unquenched lattice QCD result $1.074(18)_{\text{stat}}(16)_{\text{syst}}$ [64]. The measured slope is related to parameters of our chiral extrapolation via

$$\rho^2 = \frac{1}{\mathcal{G}(1)} \left[\rho_+^2 + \frac{r-1}{r+1} \rho_-^2 + \rho_{\text{logs}}^2 \right], \quad (4.5)$$

where ρ_{logs}^2 is the slope of the NLO logarithm at zero recoil. In Fig. 8, we compare the slope of the $B \rightarrow D$ form factor at $w = 1$ with experiment. We find $\rho^2 = 1.25(5)_{\text{stat}}$, where the error is obtained from 300 bootstrap samples. This value is in good agreement with the experimental results from Belle, CLEO, and BABAR [63] and the average of these from the Heavy Flavor Averaging Group, $\rho^2 = 1.18(6)$ [65].

Note that a determination of $\mathcal{G}(w)$ with full error budget is beyond the scope of this paper. A comprehensive effort

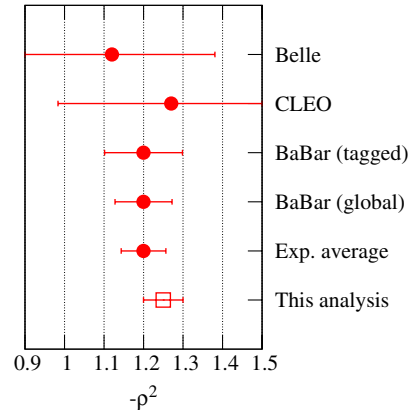


FIG. 8 (color online). The slope of the form factor $\mathcal{G}(w)$ from the chiral extrapolation is compared with various experimental measurements from Belle [77], CLEO [78], BABAR (tagged) [79], and BABAR (global) [80], respectively.

to do so is in progress [66]. Here we are merely satisfied to see that the main ingredients of our analysis are compatible with the available experimental data.

V. z PARAMETRIZATION

To minimize discretization effects, the final D meson momentum $\mathbf{p}$ should not be taken too large, so the calculations are restricted to small recoil, $w < 1.17$. However, the form-factor ratio that we are trying to compute ultimately needs to be evaluated near maximum recoil, $w \sim 1.6$, which appears to require a considerable extrapolation. Fortunately, the extrapolation can be guided by the model-independent z parametrization [25,67,68]. As shown, for example, in Ref. [69], this strategy is effective for extrapolating lattice QCD data.

One introduces the variable

$$z(w) = \frac{\sqrt{1+w} - \sqrt{2}}{\sqrt{1+w} + \sqrt{2}}, \quad (5.1)$$

which maps the physical domain of the form factors into the unit disk. The form factors can be expressed as

$$f_i(z) = \frac{1}{P(z)\phi(z)} \sum_{n=0}^{\infty} a_n z^n, \quad (5.2)$$

where $P(z)$ and $\phi(z)$ are called, respectively, the Blaschke factor and the outer function. The range of w for $B \rightarrow D$ is $1 \leq w \leq 1.589$, which corresponds to $0 \leq z \leq 0.0644$. With the choice of outer functions given below, unitarity sets a bound on the expansion coefficients,

$$\sum_n |a_n|^2 \leq 1. \quad (5.3)$$

Because of this constraint and the restricted range of z , the expansion in Eq. (5.2) converges, and one can parametrize the form factors with only a few terms. In this analysis, we truncate the expansion at the z^2 term, which is enough for our data.

Although we are primarily interested in f_0 , we apply the z expansion to f_+ and f_0 simultaneously, incorporating the kinematic constraint $f_0(0) = f_+(0)$. We take the outer functions to be

$$\phi_0(z) = \Phi_0(1+z)(1-z)^{3/2}[(1+r)(1-z) + 2\sqrt{r}(1+z)]^{-4}, \quad (5.4)$$

$$\phi_+(z) = \Phi_+(1+z)^2(1-z)^{1/2}[(1+r)(1-z) + 2\sqrt{r}(1+z)]^{-5}, \quad (5.5)$$

where we choose the constants $\Phi_0 = 0.5299$ and $\Phi_+ = 1.1213$ such that it matches the same normalization as in Ref. [67]. These exact values can be combined with the fit results, given below, to reconstitute the form factors.

The purpose of the Blaschke factor is to remove poles outside the physical region, i.e., at $w < 1$. In general,

$$P(z) = \prod_{p=1}^{N_p} \frac{z(w_p) - z(w_p)}{1 - z(w)z(w_p)}, \quad (5.6)$$

where $z(w_p)$, with $w_p = [1 + r^2 - M_p^2/M_{B(s)}^2]/2r$, marks the pole position, and the product can run over states with $M_p < M_{B(s)} + M_{D(s)}$. In the case at hand, these poles appear at the masses of $J^P = 1^-$ vector ($J^P = 0^+$ scalar) B_c mesons for $f_+(f_0)$.

We need to put the results of the chiral-continuum extrapolation in the z -parametrized form of Eq. (5.2). We do so by generating synthetic data from the chiral-continuum extrapolated curves and fitting for the corresponding parameters a_i in Eq. (5.2). Our chiral-continuum fit has 11 free parameters, including ones to describe the a^2 dependence in $h_{\pm}(w)$. Such terms vanish in the continuum limit, leaving only nine physical parameters. Furthermore, due to the small contribution from the terms of $g_{D^*D\pi}$ and $c_{0(1),+}$ and due to the correlation between $h_{\pm}(w)$, we end up with effectively six free modes in the synthetic data. Thus, we generate the synthetic data at three evenly-spaced values $w \in \{1.0, 1.08, 1.16\}$ in the region where we have data. In Sec. VIB, we show that the final form-factor ratio is not sensitive to the details of these synthetic data. We start with trivial Blaschke factors (no poles) and fit the $B \rightarrow D$ and $B_s \rightarrow D_s$ form factors up to the z^2 term in Eq. (5.2). The results of these fits are shown in Fig. 9. To examine the effect of poles on the shape of the form factor f_+ , we also try a fit with a one-pole Blaschke factor at mass $M_p = M_{B_c^*} = 6.330$ GeV, where this lowest B_c^* is a prediction of lattice QCD [70]. This Blaschke factor affects the extrapolated results with a deviation of about 0.3%. The dashed lines in Fig. 9 show the extrapolation based solely on the chiral-fit, showing that the z expansion plays an important role in controlling the total error.

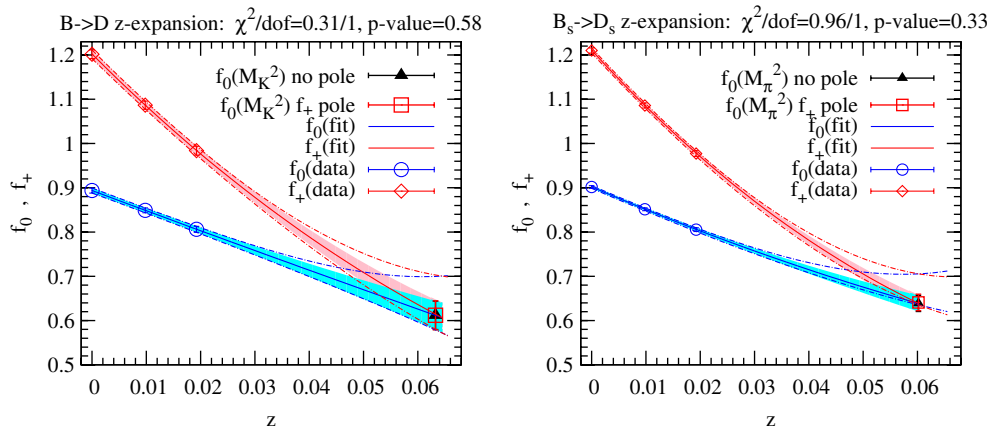


FIG. 9 (color online). z expansion of form factors to the maximum recoil point for both $B \rightarrow D$ and $B_s \rightarrow D_s$. The diamonds and circles for $z \leq 0.02$ are the synthetic data derived from the chiral-continuum extrapolation, and the solid curves and error band are the results of the z expansion. The dashed curves show how the chiral-continuum extrapolation extends into the region where the extrapolation may not be trustworthy. The points near $z = 0.06$ correspond to the desired $q^2 = M_\pi^2$ and M_K^2 ; squares (triangles) correspond to z fits with (without) the B_c^* pole in the Blaschke factor.

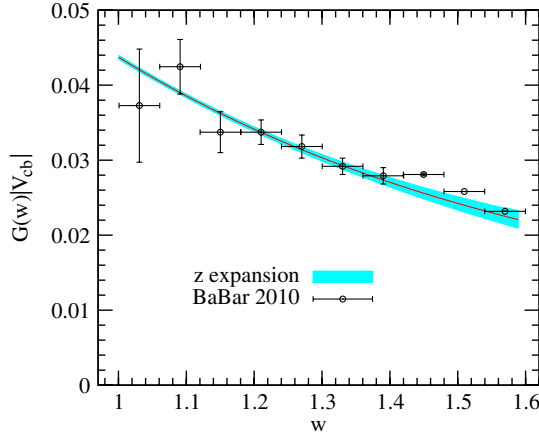


FIG. 10 (color online). Comparison of the form factor shape of $G(w)|V_{cb}|$ with *BABAR*'s measurements [71].

We perform the z -expansion fit without constraints on a_0 , a_1 , and a_2 , and setting the rest to zero. In Sec. VIB, we discuss fits with more parameters, constrained then by Eq. (5.3). We constrain the fit with the relation $f_0(0) = f_+(0)$, by demanding $|f_0(0) - f_+(0)| < \delta$ where δ can be chosen arbitrarily small. Once δ is small enough, its actual value has no effect on the fit.

To check the form factor shape obtained from the z expansion, we can compare the $B \rightarrow D$ decay with the latest published measurement from *BABAR* [71]. The comparison is shown in Fig. 10, using $|V_{cb}| = 41.4 \times 10^{-3}$, as

determined from $B \rightarrow D\ell\nu$ at nonzero recoil [71,72]. As one can see, the shape of our form factor prefers a larger value of $|V_{cb}|$ and agrees well with experiment over the full kinematic range. As above, we note that this comparison is made without a full treatment of the systematic errors on $G(w)$. A thorough treatment with full error analysis, aimed at determining $|V_{cb}|$ will be covered elsewhere; see Ref. [66] for a progress report.

For completeness, we give the results of the z fit in Table V. The correlation matrix does *not* include full systematics, but with this information the reader can reproduce the curves and error bands in Figs. 9 and 10. Note, however, that the parameters of the nonstrange and strange form factors are also correlated.

VI. SYSTEMATIC ERRORS

We now discuss the systematic errors in our analysis. Owing to the similarity between the $B \rightarrow D$ and $B_s \rightarrow D_s$ processes, the systematic errors in the ratio of the form factors largely cancel, by design. To assess the systematic uncertainties, we have repeated the chiral-continuum and z extrapolations with different choices. The values of $f_0^{(s)}(M_\pi^2)$, $f_0^{(d)}(M_K^2)$, and $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$ resulting from these variations are listed in Table VI. We summarize the final error budget in Table VII. As our standard analysis, we use Eqs. (4.1) and (4.2) for the chiral-continuum fit, dropping $c_{1,\pm}$ for $B \rightarrow D$ and $c_{0,\pm}$ for $B_s \rightarrow D_s$. We fit the

TABLE V. Best-fit values a_n and correlation matrix ρ_{mn} of the simultaneous 3-term z expansion of f_+ and f_0 , with statistical (post extrapolation) errors only. Top: $B \rightarrow D$; bottom: $B_s \rightarrow D_s$. Note that the fit parameters are correlated between the $B \rightarrow D$ and $B_s \rightarrow D_s$ processes.

$B \rightarrow D$:	0.0126(7)	-0.106(28)	0.32(66)	0.0113(5)	-0.061(26)	0.03(69)
ρ	$a_0^{(+)}$	$a_1^{(+)}$	$a_2^{(+)}$	$a_0^{(0)}$	$a_1^{(0)}$	$a_2^{(0)}$
$a_0^{(+)}$	1.000	-0.299	-0.009	0.664	-0.306	0.045
$a_1^{(+)}$		1.000	-0.231	-0.061	0.917	-0.311
$a_2^{(+)}$			1.000	-0.014	-0.164	0.976
$a_0^{(0)}$				1.000	-0.273	-0.012
$a_1^{(0)}$					1.000	-0.293
$a_2^{(0)}$						1.000
$B_s \rightarrow D_s$:	0.0119(4)	-0.111(14)	0.47(38)	0.0108(3)	-0.066(13)	0.17(41)
ρ	$a_0^{(+)}$	$a_1^{(+)}$	$a_2^{(+)}$	$a_0^{(0)}$	$a_1^{(0)}$	$a_2^{(0)}$
$a_0^{(+)}$	1.000	-0.050	-0.054	0.593	-0.067	0.038
$a_1^{(+)}$		1.000	-0.233	0.254	0.867	-0.307
$a_2^{(+)}$			1.000	0.014	-0.180	0.974
$a_0^{(0)}$				1.000	-0.055	0.002
$a_1^{(0)}$					1.000	-0.318
$a_2^{(0)}$						1.000

TABLE VI. Values of the form factors $f_0^{(s,d)}$ and their ratio for several variants of the fitting procedure. The second panel shows the results for different choices of chiral extrapolation fit function. Note that for the $B \rightarrow D$ form factor we use the fit functions labeled “val” while for the $B_s \rightarrow D_s$ form factor we use the fit functions labeled “sea” in Eqs. (6.1), (6.2), (6.3), (6.4), and (6.5). The third panel shows the results for different choices of the z expansion. The final panel shows the results for different values of parametric inputs: the lattice scale and light- and strange-quark masses.

Variations	$f_0^{(s)}(M_\pi^2)$	$f_0^{(d)}(M_K^2)$	$f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$
Standard	0.639(19)	0.612(32)	1.046(44)
(pNNLO $_{w,a,sea/val}^\pm$)			
NLO $_w^\pm$	0.636(17)	0.618(30)	1.031(42)
pNNLO $_{w,sea/val}^\pm$	0.633(18)	0.616(31)	1.030(43)
NLO $_w^+ \oplus$ pNNLO $_{w,sea/val}^-$	0.623(18)	0.594(31)	1.051(45)
With B_c^* pole in f_+	0.641(19)	0.612(33)	1.049(45)
w -Range[1,1.08]	0.623(17)	0.600(31)	1.042(42)
w -Range[1,1.12]	0.631(18)	0.606(31)	1.044(43)
w -Range[1,1.20]	0.646(19)	0.618(33)	1.048(45)
w -Range[1,1.24]	0.653(19)	0.623(34)	1.049(46)
Truncated at z^3	0.632(22)	0.607(36)	1.042(45)
Truncated at z^4	0.632(22)	0.608(36)	1.043(46)
$r_1 = 0.321$ fm	0.638(18)	0.611(32)	1.047(44)
m_s 1σ shift	0.638(18)	0.611(32)	1.046(44)
m_l 1σ shift	0.639(18)	0.612(32)	1.046(44)

TABLE VII. The error budget of the form-factor ratio discussed in text. The first row gives the statistical error after the chiral-continuum extrapolation. As explained in the text, variations in the chiral functional form make insignificant changes, so we quote no extra error for these variations. An addition discretization error for heavy-quark effects is in the last row.

Source of error	$\delta(f_0^{(s)}/f_0^{(d)})$
Statistics $\oplus$ chiral-continuum	4.2%
z expansion	0.6%
Scale r_1	0.1%
Mistuned m_s	0.1%
Mistuned m_l	0.1%
Heavy-quark (κ) tuning	0.6%
Heavy-quark discretization	1.0%

coupling $g_{D^*D\pi}$ using a constrained fit [46] with the prior 0.51(20). We take the synthetic-data points at $w = 1.0$, 1.08, and 1.16 and include the trivial Blaschke factor (no poles). We use $r_1 = 0.3117$ fm to convert the necessary physical inputs (like f_π) to r_1 units.

A. Chiral extrapolation

Our chiral extrapolation is based on the rS χ PT formalism shown in Eqs. (4.1) and (4.2) and the Appendix. The systematic errors arising here can be divided into two

categories: the error associated with the one-loop contribution itself and the error associated with the partial inclusion of NNLO analytic terms. Throughout our analysis, we keep the slope ρ^2 and curvature k , because they determine the w dependence of the form factors.

An uncertainty in the contribution from the NLO logarithm stems from the uncertainty of the $D^*-D-\pi$ coupling $g_{D^*D\pi}$. Although the NLO logarithms to $h_+(w)$ make a small contribution when evaluated with the quark masses for which we have data, of order 10^{-3} at our lightest simulated quark mass, the logarithm affects the form factor shape of $h_+(w)$ through its w dependence. Thus, the uncertainty in $g_{D^*D\pi}$ becomes more important as we extend our calculations to large recoil. We include $g_{D^*D\pi}$ in the chiral-continuum fit with the prior 0.51(20), which describes the data well, so we do not assign an additional error due to the uncertainty of $g_{D^*D\pi}$.

We now look at variations from fitting with and without the NNLO analytic terms. For ease of discussion, let us break the chiral-fitting scheme into the following different pieces:

$$\text{NLO}_w^+ = 1 - \rho_+^2(w-1) + k_+(w-1)^2 + \frac{X_+}{m_c^2} + \frac{g_{D^*D\pi}^2}{16\pi^2 f^2} \log_{1\text{-loop}}(\Lambda_\chi, w), \quad (6.1)$$

$$\text{NLO}_w^- = 1 - \rho_-^2(w-1) + k_-(w-1)^2 + \frac{X_-}{m_c}, \quad (6.2)$$

$$\text{pNNLO}_{w,\text{val}}^\pm = \text{NLO}_w^\pm + c_{0,\pm} m_\chi, \quad (6.3)$$

$$\text{pNNLO}_{w,\text{sea}}^\pm = \text{NLO}_w^\pm + c_{1,\pm}(2m_l + m_s), \quad (6.4)$$

$$\text{pNNLO}_{w,a,sea/val}^\pm = \text{pNNLO}_{w,sea/val}^\pm + c_{a,\pm} a^2, \quad (6.5)$$

where “pNNLO” stands for partial NNLO, because we include only analytic terms. We are not aware of any full NNLO calculations with nonzero final D meson momentum.

As mentioned in Sec. IV, the form factor $h_+(w)$ shows a weak dependence on the light sea- and valence-quark masses, and the data are already well-described by NLO_w^+ , with $\chi^2/\text{d.o.f.} = 0.68$ and 0.83, respectively, for $h_+^{B \rightarrow D}(w)$ and $h_+^{B_s \rightarrow D_s}(w)$. Adding the pNNLO^+ terms, the h_+ fits remain good. As seen in Figs. 6 and 7, the data for $h_-(w)$ exhibit a more significant dependence on the lattice spacing and on the sea- and spectator-quark masses. Unsurprisingly, the NLO_w^- fit of $h_-(w)$ leads to large $\chi^2/\text{d.o.f.} = 1.7$ and 1.9, respectively, for $h_-^{B \rightarrow D}$ and $h_-^{B_s \rightarrow D_s}$. The NLO χ PT correction to $h_-(w)$, denoted X_-/m_c , does not depend on quark mass or lattice spacing, so the observed dependence in the data must be described by pNNLO terms. Moving through the pNNLO functional forms in Eqs. (6.3), (6.4), and (6.5), we find that the

pNNLO $_{w,\text{val}}^-$ fit of $h^{B \rightarrow D}(w)$ improves nicely, $\chi^2/\text{d.o.f.} = 0.93$, but pNNLO $_{w,\text{sea}}^-$ fit of $h^{B_s \rightarrow D_s}(w)$ less so, $\chi^2/\text{d.o.f.} = 1.8$. These can be contrasted with the standard fits, pNNLO $_{w,a,\text{val}}^\pm$ for $B \rightarrow D$ and pNNLO $_{w,a,\text{sea}}^\pm$ for $B_s \rightarrow D_s$, with $h_- \chi^2/\text{d.o.f.} = 0.75$ and 1.6 , respectively. As seen in Table VI, these less good fits all lie well within the extrapolated statistical error of the standard fits. We therefore treat these alternatives as cross checks and do not add an additional error here.

B. z expansion

Although the z expansion provides a model-independent parametrization of the form factors f_0 and f_+ , the final results may depend on three kinds of choices made within this framework. First, the expansion coefficients may depend on the number and range of synthetic-data points. Second, the shape of the form factor may be affected by the number of poles in the Blaschke factor, particularly for f_+ . Last, the shape may be affected by the truncation of the series in z if one does not include enough terms.

To estimate the uncertainty from the synthetic data, we vary the w range over which they are generated. We repeat the z expansion with w in the intervals $[1, 1.08]$, $[1, 1.12]$, $[1, 1.20]$, $[1, 1.24]$, choosing three evenly-spaced points for both form factors. We also try fits with more synthetic data than underlying parameters, in which case some of the information is spurious, leading to tiny eigenvalues in the synthetic-data covariance matrix. We remove the corresponding mode(s) with singular-value decomposition. Although the form factors $f_0^{(d,s)}(0)$ each vary with these alternative choices by about 1σ , the ratio $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$ is negligibly affected; cf. Fig. 11. We take the maximum deviation from 1.046, which is 0.004, as the systematic error.

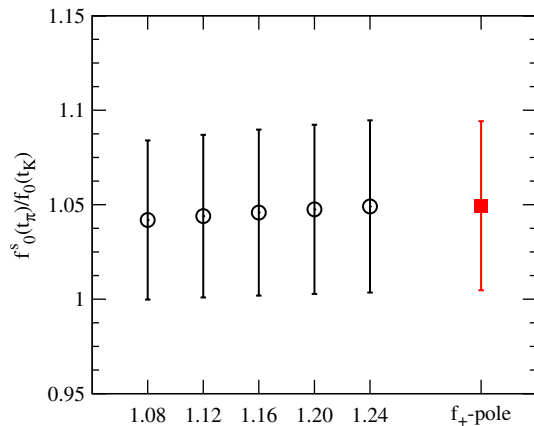


FIG. 11 (color online). Systematic error due to the z expansion. The open circles show the effect of varying the synthetic data used, and the filled square shows the effect of adding a pole to the Blaschke factor.

To estimate the uncertainty from the poles in the unphysical region, we repeat the z expansion fit by including a B_c^* pole in the Blaschke factor for f_+ . We take $M_{B_c^*} = 6.330$ GeV from a lattice QCD calculation on the MILC ensembles [70]. Recall that f_+ influences f_0 near maximum recoil via the kinematic constraint $f_0(0) = f_+(0)$. We find that the effect is rather small, as shown in Fig. 11, leading to a difference of only 0.3% in the ratio of f_0 .

To estimate the uncertainty from the truncation of higher-order terms in the z expansion, we perform the z expansion fit by including z^3 and z^4 terms and incorporating the unitarity constraints on the coefficients, i.e., $a_i^2 < 1$. As can be seen in Table VI, both the form factors and their ratios stabilize when higher-order term z^3 (or further z^4) is included. This results in a 0.3% difference in the form-factor ratio.

The total systematic error including all these effects added in quadrature is 0.6%.

C. Scale r_1 dependence

As discussed in Sec. IV, we convert our data to r_1 units with r_1/a from Ref. [24]. To convert to physical units, we must choose a value of r_1 in physical units. Our choice is based on MILC's analysis of f_π , which leads to a mass-independent value $r_1 = 0.3117(6)_{(-31)}^{(+12)}$ fm [24]. To estimate the error, we also consider an early value from HPQCD based on the 2S-1S splitting of the Υ resonances, $r_1 = 0.321(5)$ fm [73], and repeat the whole analysis with this value. We find a negligible shift, $\sim 0.1\%$, in the form-factor ratio, because of the cancellation between $B_s \rightarrow D_s$ and $B \rightarrow D$.

D. Light- and strange-quark mass dependence

The physical light- and strange-quark masses are determined from the analysis of light pseudoscalar meson masses and decay constants [28,74]. To estimate the error, we repeat the chiral-continuum extrapolation varying the masses by $\pm 1\sigma$. We do so twice, once varying the physical light-quark mass by 3.1% for $B \rightarrow D$; and again varying the physical strange-quark mass by 3.4% for $B_s \rightarrow D_s$. In both cases, we find a shift on $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$ less than 0.1%, which is much smaller than other errors in this analysis.

E. Heavy-quark mass dependence

We have not generated data for a wide-enough range of κ_b and κ_c to determine directly the heavy-quark mass dependence of the $B_s \rightarrow D_s$ form factors. Since our main focus is a U -spin breaking ratio, we rely instead on other such ratios computed on the same ensembles, in particular, the form factor for $B \rightarrow D^*$ at zero recoil $h_{A_1}(1)$ [44,75] and the ratio of leptonic decay constants f_{B_s}/f_{B^+} [76].

In the case of $h_{A_1}(1)$, which is very similar to $h_+(1)$, we find the κ -tuning error to be 0.56% of $h_{A_1}(1)$ and 4.8% of

$1 - h_{A_1}(1)$ [75]. In the case of $\xi_f = f_{B_s}/f_{B^+}$, we find the κ -tuning error to be 0.41% of ξ_f and 2.2% of $\xi_f - 1$ [76]. The first of these four estimates yields the largest absolute error on $f_0^{(s)}/f_0^{(d)}$, namely, 0.6%. This error estimate is still much smaller than the overall error in this analysis.

F. Heavy-quark mass discretization and matching

We also use our work on $h_{A_1}(1)$ [44,75] to guide and estimate heavy-quark discretization errors, both power-law and radiative effects. For $h_{A_1}(1)$, we find a 1.0% error from discretization effects and a 0.3% error from matching. Since the present calculation matches only at tree level, the corresponding errors here are order α_s instead of α_s^2 . For a U -spin breaking ratio such as ours, the discretization error is further suppressed by $(m_s - m_d)/\Lambda_{\text{QCD}}$. Since $(m_s - m_d)/(\alpha_s \Lambda_{\text{QCD}}) \sim \frac{1}{2}$, there is not much change. From the structure of Eq. (2.11), the matching error stemming from h_+ is $\alpha_s(m_s^2 - m_d^2)a^2$, which is negligible, but the matching error from h_- leads to an error on f_0 of order $\alpha_s(h_-/h_+)(m_s - m_d)/\Lambda_{\text{QCD}} \approx 0.5\%$. Taking a 1% error for these effects seems reasonable yet does not influence the total error budget much.

G. Finite-volume effects

The finite-volume correction to the function defined in Eq. (A5) in the NLO formula at zero recoil is given in Ref. [53]. Such correction was found to be very small in the $B \rightarrow D^*$ form factor [44]. One should expect similar conclusion in the case of $B_{(s)} \rightarrow D_{(s)}$. Indeed, we find that the largest effect appears at the physical light-quark masses and the magnitude of the correction is $\sim 1.0 \times 10^{-4}$ which can be safely ignored. Although the formula at nonzero recoil is not yet available, we suspect such a correction will cause any sizable effect at small recoil, considering the fact that the correction at zero recoil is 2 orders of magnitude smaller than other systematic errors. So we do not quote any systematic error from the finite-volume effects.

H. Summary

Let us now summarize our results. Table VI lists the values of $f_0^{(s)}(M_\pi^2)$, $f_0^{(d)}(M_K^2)$ and their ratio $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$ under the variations in the analysis explained above. The resulting error budget is given in Table VII, based on which, we arrive at our final result given in Eq. (1.6). The systematic error is the sum of the listed systematic errors added in quadrature. Shifting the argument of the denominator slightly and following the same analysis steps, we obtain Eq. (1.7).

VII. CONCLUSION AND DISCUSSION

To conclude, we provide the first lattice QCD calculation of the form-factor ratio $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$. Our result leads to the factor $\mathcal{N}_F = 1.094(88)(30)$, which is significantly

closer to unity than the sum-rule estimate [23], $\mathcal{N}_F^{\text{SR}} = 1.24(8)$ (or $\mathcal{N}_F^{\text{SR}} = 1.3(1)$ [19]) used in previous analyses of hadronic f_s/f_d [20,22]. As noted above, the lack of significant U -spin breaking observed in this calculation is in accord with other lattice QCD calculations of similar form factors [27].

We now examine how our new value of $\mathcal{N}_F$ affects the fragmentation-fraction ratio f_s/f_d . LHCb measures f_s/f_d via $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-)/\text{BR}(\bar{B}^0 \rightarrow D^+ K^-)$, using the sum-rule estimate $\mathcal{N}_F^{\text{SR}}$, and finds $f_s/f_d = 0.250(24)_{\text{stat}} \times (17)_{\text{syst}}(17)_{\text{theo}}$ [22]. Since $\mathcal{N}_F$ is not correlated with any other quantity in Eq. (1.3), we easily find that the fragmentation ratio should become

$$\frac{f_s}{f_d} = 0.283(27)_{\text{stat}}(19)_{\text{syst}}(24)_{\text{theo}}, \quad (7.1)$$

where the errors have also been scaled accordingly. Superficially, our theoretical error is slightly larger than that obtained with the sum-rule estimate—8.5% vs 6.5%. Our error, however, is straightforward to improve, since it is dominated by Monte Carlo statistics, propagated through the chiral-continuum and z extrapolations, as seen in Table VI.

Fleischer, Serra, and Tuning have proposed a second hadronic approach based on the ratio $\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-)/\text{BR}(\bar{B}^0 \rightarrow D^+ \pi^-)$ [20]. A complication is that a W -exchange diagram also contributes to the $\bar{B}_d^0 \rightarrow D^+ \pi^-$ decay, leading to an additional factor $\mathcal{N}_E$ in the analog of Eq. (1.3). It is estimated to be $\mathcal{N}_E = 0.966(75)$ [22]. This method requires a similar input of the form-factor ratio $\mathcal{N}'_F = [f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_\pi^2)]^2$. With our calculation, we can easily extrapolate the argument of the denominator, finding the form-factor ratio given in Eq. (1.7). As a result, $\mathcal{N}'_F = 1.111(94)(34)$. Reference [22] uses the same sum-rule value $\mathcal{N}_F^{\text{SR}} = 1.24(8)$ when doing the analysis with similar approach, finding the fragmentation-fraction ratio to be $f_s/f_d = 0.256(14)(19)(26)$. We find that

$$\frac{f_s}{f_d} = 0.286(16)_{\text{stat}}(21)_{\text{syst}}(26)_{\text{latt}}(22)_{\text{NE}}, \quad (7.2)$$

where the last two errors (major sources of the theoretical error) are shown explicitly. The last error stems from the uncertainty in $\mathcal{N}_E$. The result Eq. (7.2) agrees with that of the $D_s^+ \pi^-/D^+ K^-$ hadronic method, Eq. (7.1), and both agree with LHCb's determination via a method employing semileptonic decays, $f_s/f_d = 0.268(8)_{\text{stat}}({}_{-22}^{+24})_{\text{syst}}$ [18], as well as the Particle Data Group's average of LEP and CDF, $f_s/f_d = 0.288(24)$ [17].

As a by-product of the calculation, the form-factor ratio in Eq. (1.7) can be combined with factorization to estimate the ratio of branching ratios,

$$\frac{\text{BR}(\bar{B}_s^0 \rightarrow D_s^+ \pi^-)}{\text{BR}(\bar{B}^0 \rightarrow D^+ K^-)} = 14.4 \pm 1.3, \quad (7.3)$$

independently of experimental inputs except for quantities like $|V_{us}|f_K/|V_{ud}|f_\pi$ and lifetimes. This ratio is consistent with the measured value 16 ± 5 [17], assuming no correlation between the two processes. Smaller experimental error bars would provide a better test of the validity of our calculation.

This work is based on only 4 out of 21 available MILC asqtad ensembles of lattice-gauge configurations. Further running on ensembles closer to the chiral and continuum limits will reduce the length of the extrapolations and, hence, control the growth through extrapolation of the statistical error. At the current stage, however, the largest error in Eq. (7.1) remains experimental statistics, stemming from the difficulty in reconstructing $D_s^\pm \rightarrow KK\pi$.

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APPENDIX: STAGGERED CHIRAL PERTURBATION THEORY FOR $B \rightarrow D\ell\nu$ AT NONZERO RECOIL

The material given in the Appendix extends the continuum QCD χ PT for $B \rightarrow D\ell\nu$ [54] to staggered fermions. The staggered theory has 16 light pseudoscalar mesons for each meson of continuum QCD. Their degeneracy is broken at finite lattice spacing with masses given at the leading order by [24]

$$M_{qq'}^2 = \mu_0(m_q + m_{q'}) + a^2\Delta_\Xi, \quad (\text{A1})$$

where q, q' are the staggered quarks and μ_0 is a continuum low-energy constant. $a^2\Delta_\Xi$ are the splittings of the 16 mesons in lattice units, cf. Table III. At this order in an expansion in a^2 they come in 5 multiplets, labeled P, A, T, V , and I , with degeneracies 1, 4, 6, 4, and 1, respectively.

In full $(2+1)$ QCD rooted staggered chiral perturbation theory, we have the expression for $h_+^{B \rightarrow D}$:

$$\begin{aligned} h_+^{\text{NLO}}(w) = 1 + \frac{X_+}{m_c^2} + \frac{g_{D^*D\pi}^2}{16\pi^2 f^2} \left[\frac{1}{16} \sum_{\Xi} (2F_{\pi_\Xi}^+ + F_{K_\Xi}^+) - \frac{1}{2}F_{\pi_I}^+ + \frac{1}{6}F_{\eta_I}^+ + a^2\delta'_V \left(\frac{M_{\pi_V}^2 - M_{S_V}^2}{(M_{\pi_V}^2 - M_{\eta_V}^2)(M_{\pi_V}^2 - M_{\eta'_V}^2)} F_{\pi_V}^+ \right. \right. \\ \left. \left. + \frac{M_{\eta_V}^2 - M_{S_V}^2}{(M_{\eta_V}^2 - M_{\eta'_V}^2)(M_{\eta_V}^2 - M_{\pi_V}^2)} F_{\eta_V}^+ + \frac{M_{\eta'_V}^2 - M_{S_V}^2}{(M_{\eta'_V}^2 - M_{\eta_V}^2)(M_{\eta'_V}^2 - M_{\pi_V}^2)} F_{\eta'_V}^+ \right) + (V \rightarrow A) \right]. \end{aligned} \quad (\text{A2})$$

Similarly for $h_+^{(s)}(B_s \rightarrow D_s)$, we have

$$\begin{aligned} h_+^{(s),\text{NLO}}(w) = 1 + \frac{X_+}{m_c^2} + \frac{g_{D^*D\pi}^2}{16\pi^2 f^2} \left[\frac{1}{16} \sum_{\Xi} (F_{S_\Xi}^+ + 2F_{K_\Xi}^+) - F_{S_I}^+ + \frac{2}{3}F_{\eta_I}^+ + a^2\delta'_V \left(\frac{M_{S_V}^2 - M_{\pi_V}^2}{(M_{S_V}^2 - M_{\eta_V}^2)(M_{S_V}^2 - M_{\eta'_V}^2)} F_{S_V}^+ \right. \right. \\ \left. \left. + \frac{M_{\eta_V}^2 - M_{S_V}^2}{(M_{\eta_V}^2 - M_{\eta'_V}^2)(M_{\eta_V}^2 - M_{\pi_V}^2)} F_{\eta_V}^+ + \frac{M_{\eta'_V}^2 - M_{\pi_V}^2}{(M_{\eta'_V}^2 - M_{\eta_V}^2)(M_{\eta'_V}^2 - M_{S_V}^2)} F_{\eta'_V}^+ \right) + (V \rightarrow A) \right], \end{aligned} \quad (\text{A3})$$

where the masses of the flavor-taste singlet mesons η_I and nonsinglet mesons $\eta_{V(A)}$, $\eta'_{V(A)}$ are given by [53]

$$M_{\eta_I}^2 = \frac{1}{3}(M_{\pi_I}^2 + 2M_{S_I}^2), \quad M_{\eta_V}^2 = \frac{1}{2}(M_{\pi_V}^2 + M_{S_V}^2 + \frac{3}{4}a^2\delta'_V - Z), \quad M_{\eta'_V}^2 = \frac{1}{2}(M_{\pi_V}^2 + M_{S_V}^2 + \frac{3}{4}a^2\delta'_V + Z),$$

$$Z = \left[(M_{S_V}^2 - M_{\pi_V}^2)^2 - \frac{1}{2}a^2\delta'_V(M_{S_V}^2 - M_{\pi_V}^2) + \frac{9}{16}(a^2\delta'_V)^2 \right]^{1/2}, \quad (V \rightarrow A). \quad (\text{A4})$$

In Eqs. (A2) and (A3), F_j^+ is short for the function $F^+(w, M_j, \Delta^{(c)}/M_j)$, defined by

$$F^+(w, m, x) = -2 \left[(w+2)I_1(w, m, x) + (w^2-1)I_2(w, m, x) - \frac{3}{2}I_3(w, m, x) - \frac{3}{2}I_3(w, m, 0) \right], \quad (\text{A5})$$

where

$$I_i(w, M, x) = - \left[M^2 x E_i(w) + M^2 x^2 \ln \left(\frac{M^2}{\Lambda^2} \right) G_i(w) + M^2 x^2 F_i(w, x) \right] \quad (\text{A6})$$

and the functions E, G are given by

$$E_1(w) = \frac{\pi}{w+1}, \quad (\text{A7a})$$

$$E_2(w) = \frac{-\pi}{(w+1)^2}, \quad (\text{A7b})$$

$$E_3(w) = \pi, \quad (\text{A7c})$$

$$G_1(w) = \frac{-1}{2(w^2-1)} [w - r(w)], \quad (\text{A7d})$$

$$G_2(w) = \frac{1}{2(w^2-1)^2} [w^2 + 2 - 3wr(w)], \quad (\text{A7e})$$

$$G_3(w) = -1, \quad (\text{A7f})$$

with

$$r(w) = \frac{1}{\sqrt{w^2-1}} \ln(w + \sqrt{w^2-1}). \quad (\text{A8})$$

The functions F_i are given by

$$F_1(w, x) = \frac{1}{x^2} \int_0^{\pi/2} d\theta \frac{a}{1+w \sin 2\theta} \{ \pi(\sqrt{1-a^2}-1) - 2[f(a)-a] \}, \quad (\text{A9a})$$

$$F_2(w, x) = \frac{1}{x^2} \int_0^{\pi/2} d\theta \frac{a \sin 2\theta}{(1+w \sin 2\theta)^2} \left\{ -\frac{3\pi}{2}(\sqrt{1-a^2}-1) + \frac{\pi a^2}{2\sqrt{1-a^2}} + \frac{3-4a^2}{1-a^2} f(a) - 3a \right\}, \quad (\text{A9b})$$

$$F_3(w, x) = \frac{1}{x} \{ \pi(\sqrt{1-x^2}-1) - 2[f(x)-x] \}, \quad (\text{A9c})$$

where

$$a = \frac{x \cos \theta}{\sqrt{1+w \sin 2\theta}}, \quad (\text{A10})$$

$$f(x) = \begin{cases} \sqrt{1-x^2} \tan^{-1}[x/\sqrt{1-x^2}] & |x| < 1, \\ \frac{1}{2}\sqrt{x^2-1} \ln[1-2x(x+\sqrt{x^2-1})] & |x| > 1, \end{cases} \quad (\text{A11})$$

and $x = \Delta^{(c)}/M_j$ where M_j is the corresponding meson mass. The $D_{(s)} - D_{(s)}^*$ splittings are $\Delta^{(c)} = 140.6$ MeV, $\Delta_s^{(c)} = 143.9$ MeV. When the continuum and chiral limits are taken, the taste splittings vanish, and the 16 lowest M_j s all tend to the physical pion mass, which is around 135 MeV. The extrapolation to the physical pion mass switches from $|x| < 1$ to $|x| > 1$, requiring both expressions for $f(x)$.

- [1] A. J. Buras, *Phys. Lett. B* **566**, 115 (2003).
- [2] E. Gámiz, C. T. H. Davies, G. P. Lepage, J. Shigemitsu, and M. Wingate (HPQCD), *Phys. Rev. D* **80**, 014503 (2009).
- [3] A. J. Buras, M. V. Carlucci, S. Gori, and G. Isidori, *J. High Energy Phys.* **10** (2010) 009.
- [4] E. Golowich, J. Hewett, S. Pakvasa, A. A. Petrov, and G. K. Yeghiyan, *Phys. Rev. D* **83**, 114017 (2011).
- [5] A. J. Buras, Proc. Sci., BEAUTY 2011 (**2011**) 008 [arXiv:1106.0998].
- [6] A. G. Akeroyd, F. Mahmoudi, and D. M. Santos, *J. High Energy Phys.* **12** (2011) 088.
- [7] W. Altmannshofer and M. Carena, *Phys. Rev. D* **85**, 075006 (2012).
- [8] T. Aaltonen *et al.* (CDF), *Phys. Rev. Lett.* **100**, 101802 (2008).
- [9] V. M. Abazov *et al.* (DØ), *Phys. Lett. B* **693**, 539 (2010).
- [10] R. Aaij *et al.* (LHCb), *Phys. Lett. B* **699**, 330 (2011).
- [11] T. Aaltonen *et al.* (CDF), *Phys. Rev. Lett.* **107**, 191801 (2011).
- [12] S. Chatrchyan *et al.* (CMS), *Phys. Rev. Lett.* **107**, 191802 (2011).
- [13] R. Aaij *et al.* (LHCb), *Phys. Lett. B* **708**, 55 (2012).
- [14] S. Chatrchyan *et al.* (CMS), arXiv:1203.3976.
- [15] R. Aaij *et al.* (LHCb), arXiv:1203.4493
- [16] B. Adeva *et al.* (LHCb), arXiv:0912.4179
- [17] K. Nakamura *et al.* (Particle Data Group), *J. Phys. G* **37**, 075021 (2010).
- [18] R. Aaij *et al.* (LHCb), *Phys. Rev. D* **85**, 032008 (2012).
- [19] R. Fleischer, N. Serra, and N. Tuning, *Phys. Rev. D* **82**, 034038 (2010).
- [20] R. Fleischer, N. Serra, and N. Tuning, *Phys. Rev. D* **83**, 014017 (2011).
- [21] M. Beneke, G. Buchalla, M. Neubert, and C. T. Sachrajda, *Nucl. Phys.* **B591**, 313 (2000).
- [22] R. Aaij *et al.* (LHCb), *Phys. Rev. Lett.* **107**, 211801 (2011).
- [23] P. Blasi, P. Colangelo, G. Nardulli, and N. Paver, *Phys. Rev. D* **49**, 238 (1994).
- [24] A. Bazavov, C. Bernard, C. DeTar, Steven Gottlieb, U. M. Heller, J. E. Hetrick, J. Laiho, L. Levkova, P. B. Mackenzie, M. B. Oktay, R. Sugar, D. Toussaint, R. S. Van de Water, (MILC), *Rev. Mod. Phys.* **82**, 1349 (2010).
- [25] E. de Rafael and J. Taron, *Phys. Rev. D* **50**, 373 (1994).
- [26] D. Du, C. DeTar, A. Kronfeld, J. Laiho, Y. Meurice, S.-w. Qiu (Fermilab Lattice and MILC), Proc. Sci., LATTICE2011 (**2011**) 279 [arXiv:1111.1796].
- [27] J. Koponen, C. T. H. Davies, G. Donald, E. Follana, G. Peter Lepage, H. Na, J. Shigemitsu (HPQCD), Proc. Sci., LATTICE2011 (**2011**) 286 [arXiv:1111.0225].
- [28] E. E. Jenkins and M. J. Savage, *Phys. Lett. B* **281**, 331 (1992).
- [29] M. Neubert, *Phys. Rep.* **245**, 259 (1994).
- [30] S. Hashimoto, I. X. El-Khadra, A. S. Kronfeld, P. B. Mackenzie, S. M. Ryan, and J. N. Simone, *Phys. Rev. D* **61**, 014502 (1999).
- [31] A. S. Kronfeld, *Phys. Rev. D* **62**, 014505 (2000).
- [32] J. Harada, S. Hashimoto, K.-I. Ishikawa, A. S. Kronfeld, T. Onogi, and N. Yamada, *Phys. Rev. D* **65**, 094513 (2002).
- [33] P. Weisz, *Nucl. Phys.* **B212**, 1 (1983).
- [34] G. Curci, P. Menotti, and G. Paffuti, *Phys. Lett. B* **130**, 205 (1983).
- [35] P. Weisz and R. Wohlert, *Nucl. Phys.* **B236**, 397 (1984).
- [36] M. Lüscher and P. Weisz, *Commun. Math. Phys.* **97**, 59 (1985).
- [37] T. Blum C. DeTar, S. Gottlieb, U. M. Heller, J. E. Hetrick, K. Rummukainen, R. L. Sugar, D. Toussaint, M. Wingate, (MILC), *Phys. Rev. D* **55**, R1133 (1997).
- [38] K. Orginos, D. Toussaint, (MILC Collaboration), *Phys. Rev. D* **59**, 014501 (1998).
- [39] K. Orginos, D. Toussaint, R. Sugar, (MILC Collaboration), *Phys. Rev. D* **60**, 054503 (1999).
- [40] G. P. Lepage, *Phys. Rev. D* **59**, 074502 (1999).
- [41] J. F. Lagaë and D. K. Sinclair, *Phys. Rev. D* **59**, 014511 (1998).
- [42] B. Sheikholeslami and R. Wohlert, *Nucl. Phys.* **B259**, 572 (1985).
- [43] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, *Phys. Rev. D* **55**, 3933 (1997).
- [44] C. Bernard, C. DeTar, M. Di Pierro, A. X. El-Khadra, R. T. Evans, E. D. Freeland, E. Gamiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, M. Okamoto, J. Simone, R. Sugar, D. Toussaint, R. S. Van de Water (Fermilab Lattice and MILC), *Phys. Rev. D* **79**, 014506 (2009).
- [45] M. Wingate, J. Shigemitsu, C. T. H. Davies, G. P. Lepage, and H. D. Trottier, *Phys. Rev. D* **67**, 054505 (2003).
- [46] G. P. Lepage B. Clark, C. T. H. Davies, K. Hornbostel, P. B. Mackenzie, C. Morningstar, and H. Trottier, *Nucl. Phys. B, Proc. Suppl.* **106**, 12 (2002).
- [47] C. Morningstar, *Nucl. Phys. B, Proc. Suppl.* **A109**, 185 (2002).
- [48] W.-J. Lee and S. R. Sharpe, *Phys. Rev. D* **60**, 114503 (1999).
- [49] C. Aubin and C. Bernard, *Phys. Rev. D* **68**, 034014 (2003).
- [50] C. Aubin and C. Bernard, *Phys. Rev. D* **68**, 074011 (2003).
- [51] S. R. Sharpe and R. S. Van de Water, *Phys. Rev. D* **71**, 114505 (2005).
- [52] C. Aubin and C. Bernard, *Phys. Rev. D* **73**, 014515 (2006).
- [53] J. Laiho and R. S. Van de Water, *Phys. Rev. D* **73**, 054501 (2006).
- [54] C.-K. Chow and M. B. Wise, *Phys. Rev. D* **48**, 5202 (1993).
- [55] A. Bazavov, C. Bernard, C. DeTar, X. Du, W. Freeman, S. Gottlieb, U. M. Heller, J. E. Hetrick, J. Laiho, L. Levkova, M. B. Oktay, J. Osborn, R. Sugar, D. Toussaint, R. S. Van de Water (MILC), Proc. Sci., LATTICE2010 (**2010**) 074.
- [56] C. W. Bernard T. Burch, K. Orginos, D. Toussaint, T. A. DeGrand, C. E. DeTar, S. Gottlieb, U. M. Heller, J. E. Hetrick, and R. L. Sugar, *Phys. Rev. D* **62**, 034503 (2000).
- [57] R. Sommer, *Nucl. Phys.* **B411**, 839 (1994).
- [58] A. Anastassov *et al.* (CLEO), *Phys. Rev. D* **65**, 032003 (2002).
- [59] A. Abada, D. Becirevic, Ph. Boucaud, G. Herdoiza, J. P. Leroy, A. Le Yaouanc, O. Pene, and J. Rodriguez-Quintero, *Nucl. Phys. B, Proc. Suppl.* **119**, 641 (2003).
- [60] M. C. Arnesen, B. Grinstein, I. Z. Rothstein, and I. W. Stewart, *Phys. Rev. Lett.* **95**, 071802 (2005).
- [61] H. Ohki, H. Matsufuru, and T. Onogi, *Phys. Rev. D* **77**, 094509 (2008).
- [62] W. Detmold, C.-J. D. Lin, and S. Meinel, arXiv:1109.2480.
- [63] V. G. Lüth, *Annu. Rev. Nucl. Part. Sci.* **61**, 119 (2011).

- [64] M. Okamoto, C. Aubin, C. Bernard, C. DeTar, M. Di Pierro, A.X. El-Khadra, S. Gottlieb, E.B. Gregory, U.M. Heller, J. Hetrick, A.S. Kronfeld, P.B. Mackenzie, D.P. Menscher, M. Nobes, M.B. Oktay, J. Osborn, J.N. Simone, R. Sugar, D. Toussaint, H.D. Trotter (Fermilab Lattice and MILC), *Nucl. Phys. B, Proc. Suppl.* **140**, 461 (2005).
- [65] D. Asner *et al.* (Heavy Flavor Averaging Group), [arXiv:1010.1589](https://arxiv.org/abs/1010.1589).
- [66] S.-W. Qiu, C. DeTar, D. Du, A. S. Kronfeld, J. Laiho, R. S. Van de Water (Fermilab Lattice and MILC), *Proc. Sci., LATTICE2011* (**2011**) 289 [[arXiv:1111.0677](https://arxiv.org/abs/1111.0677)].
- [67] C. G. Boyd, B. Grinstein, and R. F. Lebed, *Nucl. Phys. B* **461**, 493 (1996).
- [68] C. G. Boyd, B. Grinstein, and R. F. Lebed, *Phys. Rev. D* **56**, 6895 (1997).
- [69] J. A. Bailey, C. Bernard, C. DeTar, M. Di Pierro, A. X. El-Khadra, R. T. Evans, E. D. Freeland, E. Gamiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, M. Okamoto, J. N. Simone, R. Sugar, D. Toussaint, R. S. Van de Water (Fermilab Lattice and MILC), *Phys. Rev. D* **79**, 054507 (2009).
- [70] E. Gregory C. T. H. Davies, E. Follana, E. Gamiz, I. D. Kendall, G. P. Lepage, H. Na, J. Shigemitsu, K. Y. Wong (HPQCD), *Phys. Rev. Lett.* **104**, 022001 (2010).
- [71] B. Aubert *et al.* (BaBar), *Phys. Rev. Lett.* **104**, 011802 (2010).
- [72] G. de Divitiis, E. Molinaro, R. Petronzio, and N. Tantalo, *Phys. Lett. B* **655**, 45 (2007).
- [73] A. Gray, I. Allison, C. T. H. Davies, E. Gulez, G. P. Lepage, J. Shigemitsu, M. Wingate (HPQCD), *Phys. Rev. D* **72**, 094507 (2005).
- [74] C. Aubin, C. Bernard, C. DeTar, S. Gottlieb, E. B. Gregory, U. M. Heller, J. E. Hetrick, J. Osborn, R. Sugar, D. Toussaint (MILC), *Phys. Rev. D* **70**, 114501 (2004).
- [75] J. A. Bailey, A. Bazavov, C. Bernard, C. M. Bouchard, C. DeTar, A. X. El-Khadra, E. D. Freeland, E. Gámiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, M. B. Oktay, J. N. Simone, R. Sugar, D. Toussaint, R. S. Van de Water (Fermilab Lattice and MILC), *Proc. Sci., LATTICE2010* (**2010**) 311 [[arXiv:1011.2166](https://arxiv.org/abs/1011.2166)].
- [76] A. Bazavov *et al.* (Fermilab Lattice and MILC), *Phys. Rev. D* (to be published).
- [77] K. Abe *et al.* (Belle), *Phys. Lett. B* **526**, 258 (2002).
- [78] J. E. Bartelt *et al.* (CLEO), *Phys. Rev. Lett.* **82**, 3746 (1999).
- [79] B. Aubert *et al.* (BaBar), [arXiv:0807.4978](https://arxiv.org/abs/0807.4978).
- [80] B. Aubert *et al.* (BaBar), *Phys. Rev. D* **79**, 012002 (2009).

***B*- and *D*-meson decay constants from three-flavor lattice QCD**

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We calculate the leptonic decay constants of $B_{(s)}$ and $D_{(s)}$ mesons in lattice QCD using staggered light quarks and Fermilab bottom and charm quarks. We compute the heavy-light-meson correlation functions on the MILC Asqtad-improved staggered gauge configurations, which include the effects of three light dynamical sea quarks. We simulate with several values of the light valence- and sea-quark masses (down to $\sim m_s/10$) and at three lattice spacings ($a \approx 0.15, 0.12$, and 0.09 fm) and extrapolate to the physical up and down quark masses and the continuum using expressions derived in heavy-light-meson staggered chiral perturbation theory. We renormalize the heavy-light axial current using a mostly nonperturbative method such that only a small correction to unity must be computed in lattice perturbation theory, and higher-order terms are expected to be small. We use the two finer lattice spacings for our central analysis, and we use the third to help estimate discretization errors. We obtain $f_{B^+} = 196.9(9.1)$ MeV, $f_{B_s} = 242.0(10.0)$ MeV, $f_{D^+} = 218.9(11.3)$ MeV, $f_{D_s} = 260.1(10.8)$ MeV, and the $SU(3)$ flavor-breaking ratios $f_{B_s}/f_B = 1.229(26)$ and $f_{D_s}/f_D = 1.188(25)$, where the numbers in parentheses are the total statistical and systematic uncertainties added in quadrature.

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I. INTRODUCTION

Leptonic decays of B and D mesons, in which the hadron annihilates weakly to a W boson, are important probes of heavy-to-light quark-flavor-changing interactions. When combined with a nonperturbative lattice QCD calculation of the heavy-light pseudoscalar meson decay constant, f_B or f_D , a precise experimental measurement of the leptonic decay width allows the determination of the Cabibbo-Kobayashi-Maskawa (CKM) quark-mixing matrix element $|V_{ub}|$ or $|V_{cd}|$. Conversely, if the relevant CKM matrix element is known from an independent process such as semileptonic decay or from CKM unitarity constraints, a comparison of the decay constant from lattice

QCD simulations with that measured by experiment provides a straightforward test of the standard model. As the lattice and experimental determinations become more precise, this test will become more sensitive and may ultimately reveal, through the appearance of a discrepancy, the presence of new physics in the quark-flavor sector.

Improved determinations of the B meson decay constant f_B are of particular importance given the current, approximately 3σ , tension in the CKM unitarity triangle that may indicate the presence of new physics in B_d mixing or $B \rightarrow \tau\nu$ decay [1–4]. The experimental uncertainty in the branching fraction $\mathcal{B}(B \rightarrow \tau\nu)$ is, at present, $\sim 30\%$ [5,6], but this error is expected to be reduced to $\sim 10\%$ at next-generation B factories KEK- B [7] with the Belle II detector [8] and Super B in Italy [9,10] in as little as five or six years, at which point even modest improvements in the

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determination of f_B will significantly help constrain the apex of the CKM unitarity triangle and isolate the source of new physics [11].

Because leptonic decays are “gold-plated” processes in numerical lattice QCD simulations (they have a single stable hadron in the initial state and no hadrons in the final state [12]), they can be determined accurately using present lattice methods. Currently, all lattice calculations of $f_{D(s)}$ and $f_{B(s)}$ that include the effects of three light dynamical quarks use staggered lattice fermions [13,14] for the up, down, and strange quarks. Because staggered fermions are computationally cheaper than other lattice fermion formulations, they allow for QCD simulations with dynamical quarks as light as $0.05m_s$, several lattice spacings, down to $a \approx 0.045$ fm, large physical volumes, and high statistics. This enables lattice determinations of many light-light and heavy-light-meson quantities with controlled systematic uncertainties. The results of staggered lattice calculations are largely in excellent numerical agreement with experimental results [12]. This includes both postdictions, such as the pion and kaon decay constants [15], and predictions, as in the case of the B_c meson mass [16]. Such successes give confidence that further calculations using the same methods are reliable. This is essential if lattice QCD calculations of hadronic weak matrix elements are to be used to test the standard model and search for new physics.

The staggered dynamical quark simulations used here employ the fourth-root procedure (“rooting”) for eliminating unwanted extra quark degrees of freedom that arise from lattice fermion doubling. The rooting method is not standard quantum field theory, and at nonzero lattice spacing it leads to violations of unitarity [17–20] that can be considered nonlocal [21]. Nevertheless, there are strong arguments [22,23] that the desired local unitary theory of QCD is reproduced by the rooted staggered lattice theory in the continuum limit. Further, one can show [18,24] that the unitarity-violating lattice artifacts in the pseudo-Goldstone boson sector can be described, and hence removed, using rooted staggered chiral perturbation theory (rS χ PT), which is a low-energy effective description of the rooted staggered lattice theory [25–27]. When coupled with other analytical and numerical evidence (see Refs. [28–31] for reviews and Ref. [32] for a recent study), this gives us confidence that the rooting procedure is valid. Indeed, the validity of the rooted staggered lattice simulations is of critical importance to flavor physics phenomenology, since a majority of the unquenched, three-flavor lattice results for hadronic weak matrix elements used to determine CKM matrix elements and as inputs to constraints on the CKM unitarity triangle come from such simulations [33].

In this paper, we present new results for the leptonic decay constants of heavy-light mesons containing bottom and charm quarks. We use the “2 + 1” flavor Asqtad-improved gauge configurations made publicly available

by the MILC Collaboration [34]. These ensembles include the effects of three light, dynamical sea-quark flavors: one with mass m_h near m_s (the physical strange-quark mass) and the other two with mass m_l as small as $0.1m_h$. We generate light valence quarks for the B and D mesons using the same staggered action as in the sea sector, and we generate heavy bottom and charm quarks using the clover action [35] with the Fermilab interpretation [36]. Because the Fermilab method uses knowledge of the heavy-quark limit of QCD to systematically eliminate heavy-quark discretization errors, exploiting ideas of Symanzik [37,38] and of heavy-quark effective theory (HQET) [39–41], it is well suited for both bottom and charm quarks. We simulate with many values for the light up/down quark mass (the mass of our lightest pion in both the sea and valence sectors is ≈ 250 MeV), and at three lattice spacings $a \approx 0.09$ fm, $a \approx 0.12$ fm, and $a \approx 0.15$ fm. We then extrapolate our numerical lattice data to the physical up and down quark masses and continuum guided by expressions derived in staggered chiral perturbation theory for heavy-light mesons (HMS χ PT) [42–44]. We try several fits of this type. Our most reliable results come from the data at $a \approx 0.09$ fm and $a \approx 0.12$ fm only. We use fits including all three lattices as part of our error analysis.

We match the heavy-light axial current to continuum QCD with a mostly nonperturbative approach, computing the flavor-diagonal (heavy-heavy and light-light) renormalization factors nonperturbatively, and then calculate the remaining flavor off-diagonal correction factor ($\rho_{A_{Qq}}^4$) in lattice perturbation theory [40,45,46]. This procedure has the advantage that $\rho_{A_{Qq}}^4$ is close to unity. Furthermore, tadpole diagrams cancel in the ratio needed to obtain $\rho_{A_{Qq}}^4$, thereby improving the convergence of the perturbative series. Empirically, the size of the one-loop contribution to $\rho_{A_{Qq}}^4$ is found to be small.

Our results for the charmed-meson decay constants improve upon our published results for f_D and f_{D_s} in Ref. [47] in several ways. The coarsest lattices used in this work have a smaller lattice spacing ($a \approx 0.15$ fm) than those used in our previous work ($a \approx 0.18$ fm). The number of configurations in the two most chiral ensembles with $a \approx 0.12$ fm has been increased, approximately by factors of 1.4 (sea $m_l = 0.1m_h$) and 1.7 (sea $m_l = 0.14m_h$). We have added new data on a new $a \approx 0.09$ fm sea-quark ensemble with a light-quark mass of $0.1m_h$. We now obtain our results from a combined analysis of our entire data set (all partially quenched mass combinations and lattice spacings). Furthermore, we now compute the bottom meson decay constants f_B and f_{B_s} . We have presented reports on this project at several conferences [48–52]; in our final analysis of this data set we also improve upon bottom and charm-quark mass-tuning, with increased statistics and a more sophisticated analysis of heavy-quark discretization effects.

This paper is organized as follows. In Sec. II, we present an overview of the calculation, including the gluon and light-quark actions used in generating the gauge configurations and the light- and heavy-quark actions used in constructing the heavy-light-meson correlators. We also introduce the mostly nonperturbative method for matching the lattice heavy-light current to the continuum and the treatment of heavy-quark discretization errors from the Fermilab action within our chiral-continuum extrapolation. Next, in Sec. III, we describe the details of our numerical simulations and we present the parameters used, such as the light-quark masses and lattice spacings. We also describe the procedure for tuning the hopping parameter in the clover action so that it corresponds to b and c quarks. In Sec. IV, we define the two-point correlation functions used to extract the decay constant at each value of the light-quark mass and lattice spacing. We use two different fitting procedures to obtain the decay constants that differ in their treatment of the statistical errors, choice of fit ranges and number of states, and choice of input correlators. We include the difference between the two in our estimate of the systematic uncertainty due to two-point fitting. Next, we present the numerical details of the calculation of the heavy-light axial-current renormalization factor in Sec. V. Putting the results of the two previous sections together, in Sec. VI, we extrapolate the renormalized decay-constant data at unphysical quark masses and nonzero lattice spacing to the physical light-quark masses and zero lattice spacing using HMS χ PT. In Sec. VII, we estimate the contributions of the various systematic uncertainties to the decay constants, discussing each item in our error budget separately. We present the final results for the decay constants in Sec. VIII, and compare them to other lattice QCD calculations and to experiment. We describe the impact of our results for current flavor physics phenomenology and then conclude by discussing the ongoing improvements to our calculations and their future impact on searches for new physics in the quark-flavor sector.

Appendix A applies HQET to the Fermilab action to obtain explicit expressions for heavy-quark discretization effects. Appendix B contains the complete set of fit results for the heavy-light pseudoscalar meson mass and renormalized decay constant for all combinations of sea-quark mass, light valence-quark mass, and heavy-quark mass used in the chiral-continuum extrapolation.

II. METHODOLOGY

The decay rate for a charged pseudoscalar meson H (with flavor content Q and $\bar{q}$) to leptons is, in the standard model,

$$\Gamma(H \rightarrow \ell \nu) = \frac{M_H}{8\pi} f_H^2 |G_F V_{Qq}^* m_\ell|^2 \left(1 - \frac{m_\ell^2}{M_H^2}\right)^2, \quad (2.1)$$

where M_H is the mass of the meson H , G_F is the Fermi constant, and V_{Qq} is the pertinent element of the CKM

matrix. The decay constant f_H parametrizes the pseudoscalar-to-vacuum matrix element of the axial-vector current,

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle = i p^\mu f_H, \quad (2.2)$$

where p^μ is the four-momentum of the pseudoscalar meson. The flavor contents of the associated vector current and CKM matrix element are given in Table I. Note that the neutral B_s decays to a charged lepton pair with an amplitude proportional to f_{B_s} ; hence the CKM factor in the decay rate involves more than one CKM matrix element. Because this process is loop suppressed in the standard model, it is potentially sensitive to new physics effects. These formulas hold for all pseudoscalar mesons; in the normalization convention used here, $f_\pi(|V_{ud}|/0.97425) = 130.41 \pm 0.20$ MeV [53].

In Eq. (2.2), the one-particle state assumes the relativistic normalization convention. For mesons containing a heavy quark, however, it is more convenient to pull out factors of M_H to ensure a smooth $M_H \rightarrow \infty$ limit:

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle (M_H)^{-1/2} = i(p^\mu/M_H) \phi_H. \quad (2.3)$$

In lattice QCD, the normalization of states on the left-hand side falls out of correlation functions more naturally. Thus, most of our analysis, including error analysis, focuses on ϕ_H . We then obtain $f_H = \phi_H/\sqrt{M_H}$ using the experimentally measured value of the meson mass [54].

To compute the decay constants with lattice gauge theory, we must choose a discretization for the heavy quark, the light quark, and the gluons. As in previous work [47,55–58], we choose the Fermilab method for heavy quarks [36] and staggered quarks with the Asqtad action [59] for the light (valence) quark. The gauge action is Symanzik improved, with couplings chosen to remove order $\alpha_s a^2$ errors from gluon loops [60], but not those from quark loops [61] (which became available only after the gauge-field generation was well underway).

For heavy bottom and charm quarks, we use the Sheikholeslami-Wohlert (SW) clover action [35] with the Fermilab interpretation [36], which connects to the continuum limit as $am_Q \rightarrow 0$. This is an extension of the Wilson action [62], which retains the Wilson action's smooth limit as $am_Q \rightarrow \infty$ and also remains well behaved for $m_Q a \approx 1$. Because this lattice action respects heavy-quark spin-flavor symmetry, one can apply HQET to

TABLE I. Flavor content of the axial-vector current and associated CKM matrix element.

H	$\mathcal{A}^\mu$	V
D	$\bar{d}\gamma^\mu\gamma^5 c$	V_{cd}^*
D_s	$\bar{s}\gamma^\mu\gamma^5 c$	V_{cs}^*
B	$\bar{b}\gamma^\mu\gamma^5 u$	V_{ub}
B_s	$\bar{b}\gamma^\mu\gamma^5 s$	—

organize the discretization effects. In essence, one uses HQET to develop the $1/m_Q$ expansion both for continuum QCD and for lattice gauge theory (LGT) [39–41]. Discretization effects are then captured order by order in the heavy-quark expansion by the difference of the short-distance coefficients in the descriptions of QCD and LGT. Thus, in principle, the lattice heavy-quark action can be improved to arbitrarily high orders in $1/m_Q$ by adjusting a sufficiently large number of parameters in the lattice action. (See Ref. [63] for details at dimensions 6 and 7. In principle, the adjustment can be done nonperturbatively, such as in the scheme of Ref. [64].) In practice, we tune the hopping parameter κ and the clover coefficient c_{SW} of the SW action, to remove discretization effects through order $1/m_Q$ in the heavy-quark expansion.

The HQET analysis of cutoff effects could be applied to any lattice action with heavy-quark symmetry, such as the action of lattice NRQCD [65]. In the latter case, it is simply a different perspective on the usual approach to lattice NRQCD, which derives the heavy-quark Lagrangian formally and then replaces derivatives with difference operators. A key feature of the Wilson, SW, Fermilab, and OK [63] actions is their well-behaved continuum limit, which is especially important for charm. For $m_Q a < 1$, one can analyze the cutoff effects in a complementary way with the Symanzik effective action [37,38]. This two-pronged attack shows that the difference of short-distance coefficients, mentioned above, vanishes as a suitable power of lattice spacing a . In this paper, we shall use our knowledge of this behavior to constrain heavy-quark discretization effects in several steps of our analysis. See Secs. III B and VI, and Appendix A for details.

The lattice and continuum currents are related by a matching factor Z_{A^μ} [40]:

$$Z_{A^\mu} A^\mu \doteq \mathcal{A}^\mu + \mathcal{O}(\alpha_s a \Lambda f_i(m_Q a)) + \mathcal{O}(a^2 \Lambda^2 f_j(m_Q a)), \quad (2.4)$$

where $\doteq$ denotes equality of matrix elements, and the functions $f_{i,j}$ that depend on $m_Q a$ stem from the difference in the HQET short-distance coefficients. In the Fermilab method, they remain of order 1 for all values of $m_Q a$ [36,63], and they are given explicitly in Appendix A. In this work, we compute Z_{A^μ} mostly nonperturbatively [45] and partly in one-loop perturbation theory. As shown in the analysis of Ref. [40], many of the Feynman diagrams in the perturbative expansion of $Z_{A_{Qq}^4}$ are common or similar to those in the flavor-conserving renormalization factors $Z_{V_{Qq}^4}$ and $Z_{V_{qq}^4}$, which can be computed nonperturbatively. Therefore, we define $\rho_{A_{Qq}^4}$ by

$$Z_{A_{Qq}^4} = \rho_{A_{Qq}^4} \sqrt{Z_{V_{qq}^4} Z_{V_{Qq}^4}}, \quad (2.5)$$

evaluating only $\rho_{A_{Qq}^4}$ in lattice perturbation theory.

The flavor-conserving factors account for most of the value of the heavy-light renormalization factor $Z_{A_{Qq}^4}$. They are obtained by enforcing the normalization condition, at zero momentum transfer,

$$1 = Z_{V_{qq}^4} \langle H_q | V_{qq}^4 | H_q \rangle, \quad (2.6)$$

where H_q is a hadron containing a single quark of flavor q , and V_{qq}^μ is the lattice version of the degenerate vector current. This condition holds for all discretizations and quark masses and, hence, the heavy quark (i.e., $Z_{V_{Qq}^4}$) as well. The remaining correction factor $\rho_{A_{Qq}^4}$ is close to unity due to the cancellation of most of the radiative corrections, including tadpole graphs. Although such cancellations have only been explicitly shown at one loop in lattice perturbation theory [40,46], we expect similar cancellations to persist at higher orders. Therefore, the perturbative truncation error in the heavy-light renormalization factor is subdominant.

III. LATTICE SIMULATION DETAILS

A. Parameters

Table II lists the subset of the ensembles of lattice gauge fields generated by the MILC Collaboration [31] used in this analysis. We now describe each entry in the table.

We analyze data at three lattice spacings: $a \approx 0.15$ fm, $a \approx 0.12$ fm, and $a \approx 0.09$ fm. The ensembles contain $2 + 1$ flavors of sea quarks, using the Asqtad-improved staggered action [59], and the square (fourth) root of the staggered determinant for the two degenerate light sea quarks (one strange sea quark). The sea contains one flavor with mass m_h close to the physical strange-quark mass and two degenerate lighter flavors of mass m_l . The tadpole improvement factor u_0 is a parameter of the gauge and Asqtad staggered (sea) quark action and is determined from the fourth root of the average plaquette. We calculate the two-point correlation functions on each ensemble from an average over four different time sources.

The relative lattice scale is determined by calculating r_1/a on each ensemble, where r_1 is related to the force between static quarks, $r_1^2 F(r_1) = 1.0$ [66,67]. Table II lists r_1/a values for each of the ensembles that result from fitting the calculated r_1/a to a smooth function [68], as explained in Eqs. (115) and (116) of Ref. [31].

In order to fix the absolute lattice scale, one must compute a physical quantity which can be compared directly to experiment. The combination of the PDG's value of f_π with MILC's 2009 determination of $r_1 f_\pi$ [69] yields $r_1 = 0.3117(6)_{-31}^{+12}$ fm. From an average of three methods for scale setting, including one based on Y splittings, the HPQCD Collaboration obtains $r_1 = 0.3133(23)(3)$ fm [70], consistent with MILC. Symmetrizing MILC's error range gives $r_1 = 0.3108(21)$ fm, and a straightforward average with the HPQCD result then yields

TABLE II. The MILC three-flavor lattices and valence Asqtad quark masses used in this work. All of the valence masses were used in version II of the correlator fits (Sec. IV C), while only the ones in bold print were used in version I (Sec. IV B).

$\approx a$ [fm]	am_h	am_l	u_0	r_1/a	$n_{\text{conf}} \times n_{\text{src}}$	Valence am_q
0.09	0.031	0.0031	0.8779	3.69	435 × 4	0.0031 , 0.0037, 0.0042, 0.0044 , 0.0052, 0.0062 , 0.0087 , 0.0124 , 0.0186 , 0.0272 , 0.031
		0.0062	0.8782	3.70	557 × 4	0.0031 , 0.0037, 0.0044 , 0.0052, 0.0062 , 0.0087 , 0.0124 , 0.0186 , 0.0272 , 0.031
		0.0124	0.8788	3.72	518 × 4	0.0031 , 0.0042 , 0.0062 , 0.0087 , 0.0124 , 0.0186 , 0.0272 , 0.031
0.12	0.05	0.005	0.8678	2.64	678 × 4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.007	0.8678	2.63	833 × 4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.01	0.8677	2.62	592 × 4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.02	0.8688	2.65	460 × 4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.03	0.8696	2.66	549 × 4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
0.15	0.0484	0.0097	0.8604	2.13	631 × 4	0.0048 , 0.007 , 0.0097 , 0.013, 0.0194 , 0.0242, 0.029 , 0.0387, 0.0484
		0.0194	0.8609	2.13	631 × 4	0.0048 , 0.007 , 0.0097 , 0.013, 0.0194 , 0.0242, 0.029 , 0.0387, 0.0484
		0.029	0.8614	2.13	576 × 4	0.0048 , 0.007 , 0.0097 , 0.013, 0.0194 , 0.0242, 0.029 , 0.0387, 0.0484

$r_1 = 0.3120(16)$ fm. This average omits likely correlations, due to the use of MILC sea-quark configurations by both groups. Conservatively assuming a 100% correlation, we inflate the error to 0.0022 fm. Finally, for convenience, we also shift the central value slightly, back to the 2009 MILC central value. We thus take $r_1 = 0.3117(22)$ fm in this paper.

The complete list of light (Asqtad) valence-quark masses m_q simulated in this analysis is also given in Table II. The mass values are selected to be roughly logarithmically spaced, but to also include the set of light sea-quark masses simulated at each lattice spacing. We use a multimass solver to compute the valence-quark propagators. The marginal numerical cost of including masses heavier than our lightest $m_q \sim 0.1 m_s$ is small, and logarithmic spacing is designed to constrain the chiral logarithms.

In Table III, we show the coefficient of the Sheikholeslami-Wohlert term c_{SW} of the clover action and the κ values used to compute heavy-light two-point functions. The coefficient of the clover term is set to the

TABLE III. Table of clover coefficients and κ values for charm and bottom used in heavy-light two-point simulations.

$\approx a$ [fm]	am_l/am_h	c_{SW}	κ_{sim} Charm	Bottom
0.09	0.0031/0.031	1.478	0.127	0.0923
	0.0062/0.031	1.476		
	0.0124/0.031	1.473		
0.12	0.005/0.05	1.72	0.122	0.086
	0.007/0.05	1.72		
	0.01/0.05	1.72		
	0.02/0.05	1.72		
	0.03/0.05	1.72		
0.15	0.0097/0.0484	1.570	0.122	0.076
	0.0194/0.0484	1.567		
	0.0290/0.0484	1.565		

tadpole-improved tree-level value $c_{\text{SW}} = u_0^{-3}$. For the $a \approx 0.09$ and 0.15 ensembles the tadpole coefficient is taken from the average plaquette. We note, however, that at lattice spacing $a \approx 0.12$ fm the tadpole coefficient u_0 appearing in both the valence Asqtad action and the heavy-quark clover action is taken from the average of the Landau link evaluated on the $am_l/am_h = 0.01/0.05$ ensemble. Hence, in our $a \approx 0.12$ fm lattice data there is a mismatch between light valence and sea quark-mass definitions. As discussed in Sec. VII, this (inadvertent) choice leads to a small error in the decay constants. We have remedied this mismatch by using the plaquette u_0 everywhere in new runs that were started while this analysis was underway.

The charm and bottom kappa values listed in Table III are based on our initial kappa tuning analysis using about one-fourth of our final statistics. We then used a larger data set to refine our determination of the κ values corresponding to bottom and charm as described in the next subsection. We adjust our data *post facto* to correspond to tuned values of κ_c and κ_b using the measured value of the derivative $\delta\phi/\delta\kappa$.

B. Input quark masses m_c and m_b

Our method for tuning κ for charm and bottom quarks closely follows that of Ref. [58], where further details can be found. We start with the dispersion relation for a heavy particle on the lattice [36],

$$E^2(p) = M_1^2 + \frac{M_1}{M_2} p^2 + \frac{1}{4} A_4 (a p^2)^2 + \frac{1}{3} A_4' a^2 \sum_{j=1}^3 |p_j|^4 + \dots, \quad (3.1)$$

where

$$M_1 \equiv E(0) \quad (3.2)$$

TABLE IV. Hopping-parameter values used to compute the dispersion relation.

$\approx a$ [fm]	$n_{\text{conf}} \times n_{\text{src}}$	κ_Q	
		Charm	Bottom
0.09	1912×4	0.1240, 0.1255, 0.1270	0.090, 0.092, 0.094
0.12	592×4	0.114, 0.117, 0.119, 0.122, 0.124	0.074, 0.086, 0.093, 0.106
0.15	631×8	0.100, 0.115, 0.122, 0.125	0.070, 0.076, 0.080, 0.090

is called the rest mass, and the kinetic mass is given by

$$M_2^{-1} \equiv \left. \frac{\partial E(\mathbf{p})}{\partial p_j^2} \right|_{\mathbf{p}=0}. \quad (3.3)$$

These meson masses differ from corresponding quark masses, m_1 and m_2 , by binding-energy effects. The bare mass or, equivalently, the hopping parameter κ must be adjusted so that these masses reproduce an experimental charmed or b -flavored meson mass. When they differ, as they do when $m_Q a \ll 1$, one must choose. Decay constants are unaffected by the heavy-quark rest mass m_1 [39], so it does not make sense to adjust the bare mass to M_1 . We therefore focus on M_2 , adjusting κ to the strange pseudo-scalars D_s and B_s , both because the signal degrades for lighter spectator masses and because this avoids introducing an unnecessary systematic uncertainty due to a chiral extrapolation.

The first step is to compute the correlator $C_2^{(S_1 S_2)}(t, \mathbf{p})$ in Eq. (4.8) (below) for several three-momenta $\mathbf{p}$, at least two light-quark masses bracketing the strange-quark mass, and several values of κ bracketing both charm and bottom. We use all momenta such that $|\mathbf{p}| \leq 4\pi/L$. Second, we fit the time dependence of the multichannel correlation matrix $C_2^{(S_1 S_2)}$ to a sum of exponentials—including the usual staggered-fermion oscillating terms—and extract the ground-state energy $aE(\mathbf{p})$ by minimization of an augmented χ^2 [58,71,72]. Third, we fit the energies to the dispersion relation given in Eq. (3.1), through $\mathcal{O}(p_i^4)$. The output of this fit is aM_1 , M_1/M_2 , A_4 , and $A_{4'}$, all as functions of κ . Fourth, we form $M_2(\kappa)$ from the first two fit outputs and r_1/a , propagating the error with a single-elimination jackknife. Finally, we obtain our tuned κ_c and κ_b by interpolating in κ so that $M_2(\kappa)$ matches the experimentally known D_s and B_s masses. The κ values used to compute M_2 are listed in Table IV. For each of the lattice spacings listed, we used the ensemble with light-to-strange sea-quark-mass ratio $am_l/am_h = 0.2$. The resulting tuned values of κ_c and κ_b are shown with errors in Table V.

We constrain the coefficients A_4 and $A_{4'}$ with Gaussian priors derived from the HQET theory of cutoff effects, adding the contribution of the priors to the χ^2 in the minimization procedure [71,72]. (In principle, we could include such priors for M_1 and M_1/M_2 too, but in practice we take priors so wide that these fit parameters are solely data driven.) Neglecting binding energies, we have exact tree-level expressions for a_4 and $a_{4'}$, the quark analogs of

A_4 and $A_{4'}$. The differences $A_4 - a_4^{[0]}$ and $A_{4'} - a_{4'}^{[0]}$ stem from both perturbative and nonperturbative effects. The asymptotics of the former can be estimated along the lines of Appendix A 3, and the latter can be deduced following the methods of Refs. [39,73]. Briefly, we constrain $A_n(\kappa)$, $n \in \{4, 4'\}$, to a Gaussian with central value

$$a_n^{[0]}(m_0 a) + \alpha_s a_n^{[1]}(m_0 a) + \bar{\Lambda} a A'_n(m_0 a). \quad (3.4)$$

Here $a_n^{[0]}$ is the exact tree-level contribution, $a_n^{[1]}$ is an estimate of the one-loop contribution, and A'_n is an expression for the binding-energy contribution. The width of the Gaussian is determined by combining in quadrature the chosen widths of the separate contributions, as outlined in Appendix A 3.

The details of the κ_c and κ_b determination differ from that of Ref. [58] in two respects. First, we use the pseudo-scalar meson masses rather than the spin average of pseudoscalar and vector meson masses, leading to a modest reduction of the statistical error. Second, we include the quartic terms in Eq. (3.1), allowing us to fold discretization effects directly into the dispersion-relation fit. Although we consider these two changes improvements, the change in the tuned κ values as compared to Ref. [58] stems primarily from the substantial increase in statistics on key ensembles.

The computations of the correlation functions needed to extract ϕ_D and ϕ_B have been carried out using the fiducial values listed in Table III. These simulation κ 's were obtained near the beginning of the project, but while the runs were in progress, we redetermined the hopping parameters utilizing increased statistics and reflecting an updated value of r_1 [69]. The resulting improved determinations

TABLE V. Hopping-parameter values κ_c and κ_b corresponding to charm and bottom. The outputs of the tuning are labeled κ_{tuned} , where the first error is from statistics and the second is from r_1 , which enters through matching to the experimentally measured D_s and B_s meson masses. The derivative $d\phi/d\kappa$ is used to correct the values of ϕ obtained with the simulated values κ_{sim} listed in Table III to the tuned values given below.

$\approx a$ [fm]	Charm		Bottom	
	κ_{tuned}	$d\phi/d\kappa$	κ_{tuned}	$d\phi/d\kappa$
0.09	0.126 91(18)(13)	−21.66	0.0959(13)(3)	−7.41
0.12	0.121 36(37)(19)	−18.23	0.0856(19)(3)	−6.82
0.15	0.120 93(36)(24)	−15.40	0.0788(11)(3)	−6.07

of κ_c and κ_b differ slightly from the simulation values. In order to adjust ϕ from the simulated value κ_{sim} to the tuned value κ_{tuned} , we write

$$\phi_{\text{tuned}} = \phi_{\text{sim}} + \frac{d\phi}{d\kappa}(\kappa_{\text{tuned}} - \kappa_{\text{sim}}), \quad (3.5)$$

where the derivatives $d\phi/d\kappa$ listed in Table V are obtained from tuning runs with nearby κ values. As explained in Sec. VII, these derivatives are also used to propagate to the decay constants the statistical and scale uncertainties on κ_{tuned} listed in Table V.

IV. TWO-POINT CORRELATOR FITS

We obtain the unrenormalized decay amplitude for every combination of heavy-quark mass, light-quark mass, and sea-quark ensemble by fitting the heavy-light-meson two-point correlation functions, described in Sec. IVA. We use two independent fitting procedures, which we refer to as “analysis I” and “analysis II.” These procedures differ in several respects. In analysis I, we use a jackknife procedure for estimating errors, while in analysis II, we use a bootstrap procedure. The two analyses also differ in their methods for handling autocorrelations in the data and in their choices of fit ranges, priors for masses and amplitudes, and number of states included. In the end, we use analysis I (Sec. IV B) to obtain central values, and we use differences from fits with different distance ranges and/or number of states included, and from analysis II (Sec. IV C) to estimate the systematic error due to choices made in the fit procedure.

A. Lattice correlators

The lattice axial-vector current is given by

$$A_a^4(x) = [\bar{\Psi}(x)\gamma^4\gamma^5\Omega(x)]_a\chi(x), \quad (4.1)$$

where $\chi(x)$ is the one-component field appearing in the staggered action, and $\Omega(x) = \gamma_1^{x_1/a}\gamma_2^{x_2/a}\gamma_3^{x_3/a}\gamma_4^{x_4/a}$ is the transformation connecting naive and staggered fields [74]. The heavy-quark field Ψ is a four-component (Dirac) spinor field, and the remaining free Dirac index is interpreted as a taste label.

To remove tree-level discretization errors in the lattice axial current, the heavy-quark field Ψ is “rotated”:

$$\Psi = [1 + ad_1\gamma \cdot D]\psi, \quad (4.2)$$

where ψ is the field appearing in the clover action. Tree-level improvement is obtained when

$$d_1 = \frac{1}{2 + m_0a} - \frac{1}{2(1 + m_0a)}, \quad (4.3)$$

where

$$m_0a = \frac{1}{u_0} \left(\frac{1}{2\kappa} - \frac{1}{2\kappa_{\text{crit}}} \right) \quad (4.4)$$

is the tapdole-improved bare mass. The critical hopping parameter κ_{crit} is the one for which the clover-clover pion mass vanishes.

As usual in lattice gauge theory, we obtain the matrix element in (2.3) from two-point correlation functions. We introduce pseudoscalar operators

$$\mathcal{O}_a^{(S)}(x) = \sum_y [\bar{\psi}(y)S(y, x)\gamma^5\Omega(x)]_a\chi(x), \quad (4.5)$$

depending on a “smearing” function S . In this work, we use two functions, the local (or unsmeared) source $S(x, y) = \delta_{xy}$ and the smeared source (in Coulomb gauge)

$$S(x, y) = \delta_{x_4y_4}S(\mathbf{x} - \mathbf{y}), \quad (4.6)$$

where $S(\mathbf{r})$ is the 1S solution of the Richardson potential for the quarkonium systems [75]. We obtain $S(\mathbf{x} - \mathbf{y})$ by scaling the radial Richardson wave function to lattice units, interpolating it to lattice sites, and then using it as the spatial source for the heavy-quark propagators [76].

We introduce two-point correlation functions

$$\Phi_2^{(S)}(t) = \sum_{a=1}^4 \sum_{\mathbf{x}} \langle A_a^{4\dagger}(t, \mathbf{x}) \mathcal{O}_a^{(S)}(0) \rangle, \quad (4.7)$$

$$C_2^{(S_1S_2)}(t, \mathbf{p}) = \sum_{a=1}^4 \sum_{\mathbf{x}} e^{i\mathbf{p} \cdot \mathbf{x}} \langle \mathcal{O}_a^{(S_1)\dagger}(t, \mathbf{x}) \mathcal{O}_a^{(S_2)}(0) \rangle, \quad (4.8)$$

where $\langle \bullet \rangle$ now represents the ensemble average. For large time separations, $\Phi_2^{(S)}$ is proportional to the matrix element ϕ_H , and the proportionality is determined from $C_2^{(SS)}(t, 0)$. Each two-point function is constructed from a staggered quark propagator with local (δ) sources and sinks. We compute C_2 functions for all (four) combinations $S_1, S_2 = \delta$ and 1S, requiring heavy clover-quark propagators with all combinations of 1S smeared and local sources and sinks. Only the local sink clover propagators are needed to compute the Φ_2 functions. With the sum over tastes in Eqs. (4.7) and (4.8), the correlation functions Φ_2 and C_2 can also be cast in a heavy-naive formalism [77].

The staggered light quarks in the axial-current and pseudoscalar two-point correlation functions lead to the presence of opposite-parity states that oscillate in time as $(-1)^t$. Hence the two-point functions take the following forms:

$$\begin{aligned} \Phi_2^{(S)}(t) = & A_{\Phi}^{(S)}(e^{-Mt} + e^{-M(T-t)}) \\ & + \tilde{A}_{\Phi}^{(S)}(-1)^t(e^{-\tilde{M}t} + e^{-\tilde{M}(T-t)}) \\ & + A_{\Phi}^{\prime(S)}(e^{-M't} + e^{-M'(T-t)}) + \dots, \end{aligned} \quad (4.9)$$

$$\begin{aligned} C_2^{(S_1S_2)}(t, \vec{p} = 0) = & A^{(S_1)}A^{(S_2)}(e^{-Mt} + e^{-M(T-t)}) \\ & + \tilde{A}^{(S_1)}\tilde{A}^{(S_2)}(-1)^t(e^{-\tilde{M}t} + e^{-\tilde{M}(T-t)}) \\ & + A^{\prime(S_1)}A^{\prime(S_2)}(e^{-M't} + e^{-M'(T-t)}) + \dots, \end{aligned} \quad (4.10)$$

where a prime denotes a standard excited state of the same parity and a tilde denotes the mass or amplitude of an opposite-parity state. The oscillating behavior is visible throughout the entire lattice temporal extent and must be included in fits to extract the ground-state mass and amplitudes.

We then obtain the renormalized decay amplitude in lattice units from the ratio

$$a^{3/2}\phi_H = \sqrt{2} \frac{Z_{A_{\phi q}^4} A_{\phi}^{(S)}}{A^{(S)}}, \quad (4.11)$$

where $A_{\phi}^{(S)}$ and $A^{(S)}$ are the amplitudes of the ground-state exponentials defined in Eqs. (4.9) and (4.10), and the renormalization factor $Z_{A_{\phi q}^4}$ is discussed in Sec. V.

B. Analysis I

Our primary analysis of two-point correlation functions $\Phi_2^{(S)}$ and $C_2^{(S_1 S_2)}$ —analysis I—proceeds as follows. The amplitudes $A_{\phi}^{(S)}$ and $A^{(S)}$ in Eq. (4.11) are determined from fits to multiple correlators using the full data correlation matrix. In analysis I, we start by fitting combinations A, B, C, and D in Table VI. We find combination A, which uses the axial-current correlator with a 1S smeared source and the pseudoscalar correlator with a 1S smeared source and sink, to be suitable. The extra complexity of combinations of three correlators (C and D) gives little benefit, and the errors from combination A are somewhat smaller than those from combination B.

For fits to charm-light-meson correlators, we include just one simple exponential (the desired state) and one oscillating exponential, which we call a “1 + 1 state fit.” We choose the minimum distance $t_{\min}$ such that contributions from excited states are small compared to our statistical errors. Because we fit two propagators simultaneously while imposing the constraint that the masses be equal, this is a six-parameter fit: two amplitudes for each propagator and a common mass for each of the simple and oscillating exponentials. To help stabilize the fit, the amplitudes and

TABLE VI. Combinations of two-point functions that can be used to extract $a^{3/2}\phi_H$. All combinations of two and three correlators are shown. Additional combinations of four or more correlators are not enumerated.

Two-point function	Fit combination					
	A	B	C	D	E	F
$\Phi_2^{(1S)}(t)$	•		•	•	•	•
$\Phi_2^{(\delta)}(t)$		•	•	•	•	•
$C_2^{(1S,1S)}(t)$	•				•	•
$C_2^{(\delta,\delta)}(t)$		•			•	
$C_2^{(\delta,1S)}(t)$			•			•
$C_2^{(1S,\delta)}(t)$				•		

mass of the oscillating state are weakly constrained by Gaussian priors, which are incorporated as additional terms in χ^2 in the fitting procedure [71,72]. The central values for these priors are determined by a trial fit, where the prior for the opposite-parity mass is set to 500 ± 250 MeV above the ground-state mass,¹ and the amplitudes are unconstrained. Then the jackknife fits use central values for the opposite-parity state amplitudes and mass determined by the trial fit, with Gaussian widths that are typically 3–10 times the error estimates on these parameters, so in the end the priors make a negligible contribution to χ^2 . We have checked, by varying the prior widths for three of the 0.09 fm ensembles, that such wide priors are still narrow enough to ensure stable fits. We propagate the uncertainties in the correlator fits to the subsequent chiral-continuum extrapolation with a jackknife procedure. In the jackknife resamples, we center the priors at the values found in the fit to the full ensemble, again with widths that are typically 3–10 times the error estimates on these parameters.

The bottom meson correlators fall off much more rapidly with t , so it is difficult to take a large enough minimum distance to ensure that excited state contributions are negligible. Therefore, we use a fit with two simple exponentials and one oscillating exponential, or a “2 + 1 state fit.” The mass of this excited state is also weakly constrained by priors in the same way that the opposite-parity mass is, except that the width of the prior on the excited state mass is set to 200 MeV.

Figure 1 shows the heavy-light pseudoscalar mass as a function of the minimum time used in the fit. The left-hand plots show sample fits to bottom correlators, while the right-hand plots show sample fits to charm correlators. We select fitting ranges to give reasonable fits for all sea-quark ensembles and all valence-quark masses. We quantify the goodness of fit with the “ p value” [54], which is the probability that a fit with this number of degrees of freedom would have a χ^2 larger than this value. Table VII gives the fit ranges for charm-light and bottom-light correlators on the three lattice spacings, both for the fits used for the central values and for alternate fits used in estimating systematic errors from choices of fit parameters. The meson masses, $a^{3/2}\phi_H$ values, and p values for the data set used in analysis I are tabulated in Appendix B.

The decay amplitude $a^{3/2}\phi_H$ is highly correlated among different light valence-quark masses on the same ensemble. To propagate the correlations among the different valence masses to the subsequent chiral-continuum extrapolation, in Sec. VI, we use a single-elimination jackknife procedure to estimate the covariance matrix of $a^{3/2}\phi_H$ for the selected valence-quark masses. This

¹Although 500 MeV is a reasonable guess for the mass gap to the first excited state of the meson, we actually expect that this excited state in the fit approximates the contributions of a number of physical states, likely including both single-particle and multiparticle channels.

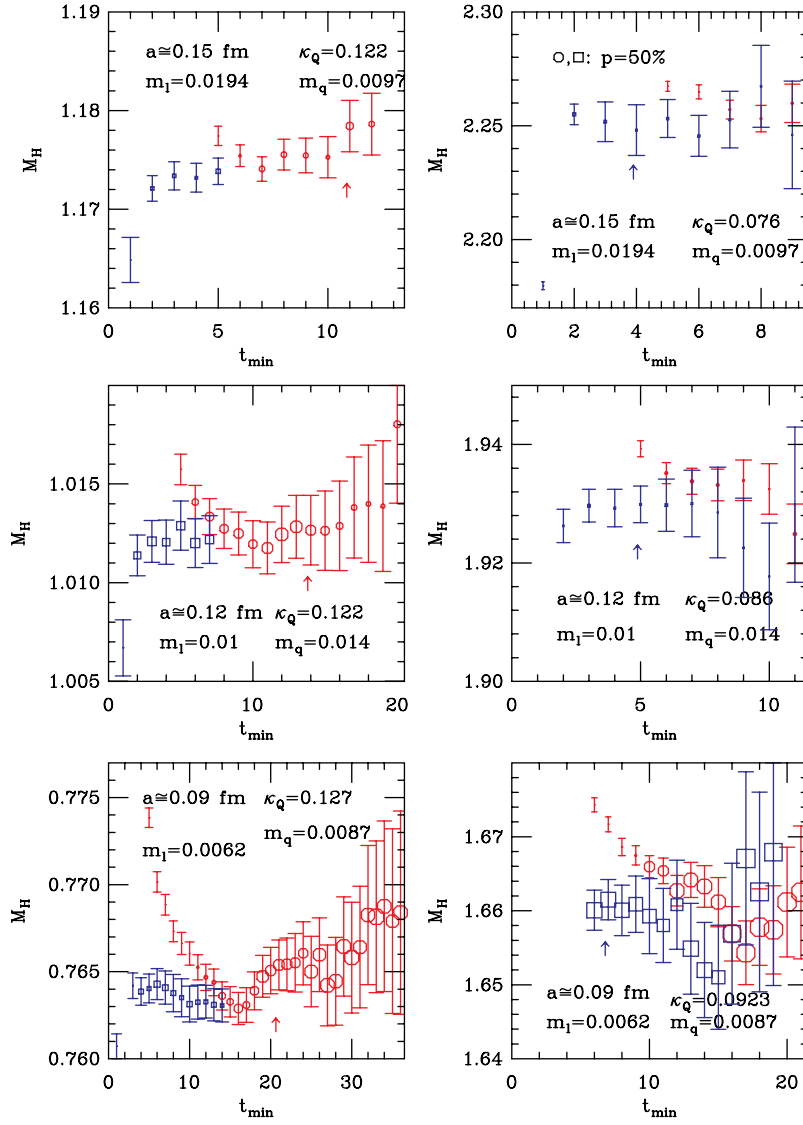


FIG. 1 (color online). Ground-state rest mass M_H versus minimum distance $t_{\min}$ included in the fit. For each lattice spacing, we show an ensemble with the dynamical light-quark mass m_l in the middle of the range. Similarly, we show correlators with a valence-quark mass m_v in the center of the ranges used. The top two panels are at $a \approx 0.15$ fm, the middle two at $a \approx 0.12$ fm, and the bottom two at $a \approx 0.09$ fm. In each row the left panel shows results for charm and the right-panel shows results for bottom. The size of each plot symbol is proportional to the p value (confidence level) of the fit, with the symbol size in the legends of the upper right panel corresponding to $p = 50\%$. The red octagons are for fits including one state of each parity (“1 + 1 fits”), and the blue squares are for fits including an excited state of the same parity as the ground state (“2 + 1 fits”). In each panel, the arrow indicates the fit that is used in Sec. VI.

is done by computing the covariance matrix of the single-elimination jackknife samples, and multiplying by $(N - 1)^2$, where N is the number of configurations in the ensemble. In fact, when all valence-quark masses are kept, the covariance matrices are close enough to singular to be unmanageable. This reflects the fact that the correlators for intermediate valence masses can be very accurately predicted from the correlators for nearby masses, so some of the correlators provide very little new information. Therefore, we omit some valence-quark masses, using only those set in bold in Table II.

We use a single-elimination jackknife rather than an omit- J jackknife because a large number of samples are needed to compute a reliable covariance matrix. Successive configurations in the ensemble are not independent, however, so we must take autocorrelations into account. We do so by repeating the calculation after first blocking the data by a factor of 4. (This block size of 4 is determined from tests on the $a \approx 0.12$ fm lattices using fit analysis II, for which it gives a reasonable compromise between suppressing autocorrelations and leaving enough data points for the statistical analysis.) We then compute,

TABLE VII. Numbers of states and time ranges used in two-point analysis I. In the number of states, “1 + 1” means one simple exponential and one oscillating state (opposite parity). The fits in columns two through five were used for the central values, while the fits in columns six through nine were used in estimating systematic errors from the choice of fit ranges (see Sec. VIIC).

$\approx a$ [fm]	Central fits				Alternate fits			
	Charm		Bottom		Charm		Bottom	
	n_{states}	t range	n_{states}	t range	n_{states}	t range	n_{states}	t range
0.15	1 + 1	11–23	2 + 1	4–20	1 + 1	12–23	1 + 1	9–20
0.12	1 + 1	14–31	2 + 1	5–22	1 + 1	16–31	1 + 1	12–22
0.09	1 + 1	21–47	2 + 1	7–30	1 + 1	23–47	1 + 1	16–30

for each valence-quark mass i , the ratio R_i of the diagonal element of the covariance matrix with a block size of 4 to the same element of the unblocked covariance matrix:

$$R_i = \sigma_{ii}^{(4)} / \sigma_{ii}, \quad (4.12)$$

where the superscript denotes the block size. The rescaled covariance matrix for $a^{3/2}\phi_H$ is given by

$$C_{ij}^{(4)} = C_{ij} \sqrt{R_i R_j}, \quad (4.13)$$

which preserves the eigenvalue structure of the covariance matrix, whereas simply using the covariance matrix of the blocked data would be more likely to produce spurious small eigenvalues. The rescaling factors R_i themselves have errors, and in many cases turn out to be less than 1. In such cases, we do not replace the R_i by 1, despite the fact that this would likely be a better estimate of the individual R_i . Doing so would yield a covariance matrix with a bias toward larger errors and could produce misleading estimates of goodness of fit in the later analysis.

Finally, we combine the covariance matrices from all of the individual ensembles into larger covariance matrices, one each for the charm and bottom $a^{3/2}\phi_H$. Since different ensembles are statistically independent, these large covariance matrices are block diagonal, with each block containing the correlations among different light valence-quark masses on a single sea-quark ensemble.

C. Analysis II

Analysis II is a second, independent analysis of the two-point correlators that uses the bootstrap method to propagate correlated errors from the two-point analysis through to the chiral extrapolations. In analysis II, we block average the two-point correlator data over four sequential configurations (which themselves are spaced by more than four trajectories) before the analysis. In the bootstrap procedure, we resample the data (with replacement), taking the number of sampled configurations to be equal to the number of blocked configurations in each bootstrap ensemble. For each bootstrap ensemble, we recompute the covariance matrix. During the bootstrap process, we randomly draw from a Gaussian distribution new prior

mean values of each constrained parameter belonging to an excited state while keeping the widths fixed. The ground-state parameters are given loose priors so that the fitted values are determined by the data. To help stabilize the fits, the ground-state prior means are not randomized in the bootstrap. Prior values for the energy splittings are taken from a chiral quark model calculation for the D and B meson systems [78]. Prior widths are taken to be about 200 MeV for excited states. Excited state amplitudes $\log(A^{(S)})$ have a prior width $\sigma_{\log A} = 2$.

On each gauge ensemble, the same sequence of gauge resamplings is taken for all valence m_q to preserve correlations among $a^{3/2}\phi_H$ values. Our final results are based upon 4000 bootstrap replications of the data. We use the central values of $a^{3/2}\phi_H$ from the fits to the entire ensemble in the chiral-continuum extrapolation, and we use the bootstrap values to obtain the covariance matrix.

To optimize the determination of $a^{3/2}\phi_H$, we compare simultaneous fits of up to six two-point functions; the various combinations of up to four functions are listed in Table VI. At a minimum, one axial-current correlator must be paired with one propagator (combinations A or B in Table VI) to extract $a^{3/2}\phi_H$. Combination A, using smeared operators, is used in analysis I, described above. Because fits of four or more two-point functions over a wide time range can lead to a poorly determined data covariance matrix having large rank relative to the number of available configurations, we focus on combinations having two or three correlators. Unlike combination A, combination B does not take advantage of smeared sources, and the ratio does not show convincing plateaus over the range of times with decent signal-to-noise ratios. Comparing combination C to D, the smeared source in C is less noisy than the smeared sink in D.

Given these considerations, for fits to charm correlators, we use the two-point function combination C to obtain $a^{3/2}\phi_H$, which uses both of the axial-current functions. We look for stability of the ground-state mass and amplitude when varying $t_{\min}$, $t_{\max}$, and the number of excited states included in the fit. We also compare fit results from other combinations of correlators to check that we have isolated the correct ground-state energy and matrix element. Our

final results come from fits accounting for two pseudoscalar states and two (oscillating) opposite-parity states.

For fits to bottom correlators, we use combination B for our final results; this is the same set used in analysis I. Combination C gives fits with rather low confidence levels for the B meson and tends to result in larger errors for $a^{3/2}\phi_H$. Again, we examine fits varying the time range; we also try fits with up to three pseudoscalar states plus three oscillating opposite-parity states. We use these fits and fits to alternate combinations of two-point correlators as a consistency check.

The fit results from the two different analyses are consistent with each other for most cases, but there are a few cases where they differ by a standard deviation or more (see Fig. 11). The $a^{3/2}\phi_H$ results from the two analyses are propagated through the chiral-continuum extrapolations in Secs. VIB and VIC. The resulting differences in the extrapolated results in turn provide the basis for our systematic error analysis due to fit choices given in Sec. VIIC.

V. HEAVY-LIGHT CURRENT MATCHING

In this section, we discuss in more detail the ingredients of Eq. (2.5), which allow a “mostly nonperturbative” matching procedure [45].

A. Perturbative calculation of $\rho_{A_{Qq}^4}$

The perturbative expansion of $\rho_{A_{Qq}^4}$ can be written as

$$\rho_{A_{Qq}^4} = 1 + \alpha_s(q^*)\rho_{A^4}^{[1]}(m_Q a, m_q a) + \dots \quad (5.1)$$

where α_s is the strong coupling and $\rho_{A^4}^{[1]}$ is the one-loop coefficient. The one-loop coefficient is calculated in Ref. [46] using lattice perturbation theory, where we see explicitly that $\rho_{A^4}^{[1]}$ is small because most of the one-loop corrections cancel. The self-energy contributions cancel exactly (to all orders, in fact), and, in practice, we are in a region where $\rho_{A^4}^{[1]}(m_Q a, m_q a)$, viewed as a function of $m_Q a$, has two zeros. Therefore, the renormalization factor $\rho_{A_{Qq}^4}$ is close to unity for both bottom and charm.

The perturbative calculation of $\rho_{A_{Qq}^4}$ in Eq. (5.1) proceeds as follows. We use $\alpha_s(q^*)$ defined in the V scheme [79] as determined in Ref. [80], and take $q^* = 2/a$, which is close to the optimal choice of Refs. [79,81] for a wide range of quark masses. The one-loop coefficients $\rho_{A^4}^{[1]}$ are computed for light-quark masses $am_q = 0.001, 0.01, 0.04$ to cover the range used in this analysis. From these we obtain $\rho_{A_{Qq}^4}$ at other light-quark masses by linear interpolation in am_q . For illustration, Table VIII lists $\rho_{A_{bq}^4}$ and $\rho_{A_{cq}^4}$ evaluated at the light valence mass $am_q = 0.01$ for the 11 sea-quark ensembles used in this work. Note that the sea-quark-mass dependence is indirect, via the plaquette used to determine $\alpha_s(q^*)$. The dependence on the light-quark

TABLE VIII. The perturbative correction factor $\rho_{A_{Qq}^4}$ for the heavy-light current A^4 at the simulated charm and bottom heavy-quark κ values given in Table III and at $am_q = 0.01$ for the different sea-quark ensembles. The statistical errors associated with the numerical integration are negligible.

$\approx a$ [fm]	am_l/am_h	$\rho_{A_{bq}^4}$	$\rho_{A_{cq}^4}$
0.09	0.0031/0.031	1.0026	1.0000
	0.0062/0.031	1.0026	1.0000
	0.0124/0.031	1.0026	1.0000
0.12	0.005/0.05	1.0081	0.9959
	0.007/0.05	1.0081	0.9959
	0.010/0.05	1.0081	0.9959
	0.020/0.05	1.0080	0.9960
	0.030/0.05	1.0079	0.9961
0.15	0.0097/0.0484	1.0270	0.9937
	0.0194/0.0484	1.0267	0.9938
	0.0290/0.0484	1.0265	0.9938

mass in the current is very mild: for bottom, $\rho_{A_{bq}^4}$ changes with am_q by 0.07–0.2%, depending on lattice spacing, and for charm, $\rho_{A_{cq}^4}$ changes by around 0.1%. On the fine ensembles, the am_q dependence is almost as large as the total one-loop correction because the overall cancellation, especially in $\rho_{A_{cq}^4}$, is so fortuitously good.

B. Nonperturbative computation of $Z_{V_{qq}^4}$ and $Z_{V_{Qq}^4}$

The nonperturbative part of the matching factor $Z_{A_{Qq}^4}$ is obtained from the temporal components of the clover-clover and staggered-staggered vector currents. At zero momentum transfer, the (correctly normalized) vector current simply counts flavor number, so it is possible to obtain Z_{V^4} nonperturbatively for any discretization and any mass [45].

For the staggered-staggered current, we compute

$$C_3^{(S_1 S_2)}(t_2, 0, t_1) = \sum_{ab} \sum_{x,y} \langle \mathcal{O}_a^{(S_1)}(t_2, y) V_{ab}^4(0) \mathcal{O}_b^{(S_2)\dagger}(t_1, x) \rangle, \quad (5.2)$$

where, as in Eq. (4.5), $\mathcal{O}_a^{(S)}$ is a smeared or local clover-staggered meson operator with mass chosen to optimize the signal, and

$$V_{ab}^4(x) = \bar{\chi}(x) [\Omega^\dagger(x) \gamma^4 \Omega(x)]_{ab} \chi(x) \quad (5.3)$$

is the temporal component of the staggered-staggered vector current. The three-point functions C_3 are computed from the same staggered quarks used for the clover-staggered two-point functions. The staggered quark is transformed into an improved naive quark by applying the Ω matrix; this naive quark at time t_1 is then used as the source term when computing the charm propagator. We smear the source at t_1 so that $S_1 = S_2$.

We compute $Z_{V_{qq}^4}$ using a D_q meson [cf. Eq. (4.5)], which provides a good signal. The three-point function $C_3^{(S_1 S_2)}(t_2, 0, t_1)$ contains states of both the desired and the opposite parity, with the latter carrying oscillating $(-1)^t$ dependence. We construct $C_3^{(S_1 S_2)}(t_2, 0, t_1)$ with local sources $S_1 = S_2 = \delta$ and compute it at multiple even and odd values of t_1 and t_2 in order to disentangle the ground-state amplitude from the other contributions.

Within the time range $t_1 < 0 < t_2$ and in the limit of large separations, $|t_1|, t_2 \gg a$,

$$\begin{aligned} C_3^{(\delta, \delta)}(t_2, 0, t_1) = & Z_{V_{qq}^4}^{-1} A^2 \exp(-E(t_2 - t_1)) \\ & + Z' AB [(-1)^{t_1} \exp(E' t_1 - E t_2) \\ & + (-1)^{t_2} \exp(E t_1 - E' t_2)] \\ & + Z'' B^2 (-1)^{(t_1 + t_2)} \exp(-E'(t_2 - t_1)) + \dots, \end{aligned} \quad (5.4)$$

neglecting contributions from excited states. We extract $Z_{V_{qq}^4}$ from a minimum χ^2 fit to the three-point function using the right-hand side of Eq. (5.4) as the model function. The fit is linear in the free parameters $Z_{V_{qq}^4}^{-1}$, Z'' , and Z' , while we fix the ground-state energies E and E' , and the operator overlaps A and B to the values determined by fitting the two-point function $C_2^{(\delta)}(t, 0)$. We use a single-elimination jackknife procedure to compute the data covariance matrix.

Table IX presents our results for $Z_{V_{qq}^4}$ on the ensembles used in this work. The three-point functions for the $Z_{V_{qq}^4}$ calculation are generated at a single source time, $t_{\text{src}} = 0$ (instead of the four used for two-point functions $\Phi_2^{(S)}$ and $C_2^{(S_1 S_2)}$). At $a \approx 0.12$ fm we have results at two values of the sea-quark masses which are consistent within errors. At $a \approx 0.09$ and 0.15 fm we have results for several values of m_q . We do not see evidence for a dependence upon m_q with current statistics. The errors, however, increase at smaller

quark mass. Hence, we use the $Z_{V_{qq}^4}$ corresponding to $m_q \sim m_s$ in Eq. (4.11). In the table, they are set in *bold*.

For the clover-clover current, we compute

$$\tilde{C}_3^{(S_1 S_2)}(t_2, t_1, 0) = \sum_{x, y} \langle \tilde{\mathcal{O}}^{(S_1)^\dagger}(t_2, y) V_{QQ}^4(t_1, x) \tilde{\mathcal{O}}^{(S_2)}(0) \rangle, \quad (5.5)$$

where

$$V_{QQ}^4(x) = \bar{\Psi}(x) \gamma^4 \Psi(x) \quad (5.6)$$

is the temporal component of the (rotated) clover-clover vector current. The clover-clover bilinear

$$\tilde{\mathcal{O}}^{(S)}(x) = \sum_y \bar{\psi}(y) S(x, y) \gamma^5 s(x) \quad (5.7)$$

consists of a heavy-quark field corresponding to charm or bottom, as the case may be, and a light clover-quark field s with mass chosen to provide a good signal. At large time separations, these three-point functions are proportional to $Z_{V_{QQ}^4}^{-1}$, with the proportionality coming from

$$\tilde{C}_2^{(S_1 S_2)}(t) = \sum_x \langle \tilde{\mathcal{O}}^{(S_1)^\dagger}(t, x) \tilde{\mathcal{O}}^{(S_2)}(0) \rangle. \quad (5.8)$$

We compute $Z_{V_{QQ}^4}$ using a $\bar{Q}s$ meson, where the strange quark is simulated with the clover action to circumvent oscillating opposite-parity states [cf. Eq. (5.7)]. We restrict our calculation of $\tilde{C}_{2,3}$ to $S = S_1 = S_2$ using both local and $1S$ smearing functions. The function $\tilde{C}_2$ combines a local-local clover quark with mass around m_s and a heavy clover-quark propagator with source and sink S . The function $\tilde{C}_3$ requires the same heavy- and light-quark propagators as needed in $\tilde{C}_2$. An additional heavy-quark propagator originating from t_2 has as its source the light-quark propagator restricted to t_2 , multiplied by γ_5 and convolved with the smearing function S .

In Eq. (5.7), we use a random color wall source with three dilutions for both the heavy and light spectator quarks that originate from $t = 0$. We generate two- and three-point functions for both local-local and smeared-smeared

TABLE IX. Light-light vector current renormalization factor $Z_{V_{qq}^4}$. Values in bold are used in computing the heavy-light current renormalizations. With our conventions, the tree-level value of $Z_{V_{qq}^4}$ is 2. A colon is used to represent the range of time values included in the fit.

$\approx a$ [fm]	am_l/am_h	n_{conf}	$-t_1$	t_2	am_q	$Z_{V_{qq}^4}$
0.09	0.0124/0.031	518	23:12	11:13	0.0272	1.868(49)
			23:12	11:13	0.0124	1.883(69)
0.12	0.01/0.05	592	15:9	7:11	0.03	1.853(45)
	0.007/0.05	523	20:7	7:12	0.03	1.882(56)
0.15	0.0097/0.0484	631	20:5	4:12	0.0484	1.704(34)
			20:5	4:12	0.029	1.709(40)
			20:5	4:12	0.0242	1.711(42)
			20:5	4:12	0.0194	1.707(45)
			20:5	4:12	0.0097	1.662(55)

TABLE X. Heavy-heavy vector current renormalization factor $Z_{V_{\bar{q}q}^4}$ computed at several κ values, covering the charm and bottom quark masses, for three lattice spacings.

$\approx a$ [fm]	am_l/am_h	$n_{\text{conf}} \times n_{\text{src}}$	κ_Q	$Z_{V_{\bar{q}q}^4}$
0.09	0.0062/0.031	1912×2	0.1283	0.2749(4)
			0.127	0.2830(4)
			0.110	0.3856(6)
			0.0950	0.4730(8)
			0.0931	0.4840(9)
0.12	0.007/0.05	2110×2	0.124	0.2899(4)
			0.122	0.3028(4)
			0.116	0.3410(5)
			0.098	0.4507(7)
			0.086	0.5209(10)
0.15	0.0194/0.0484	631×2	0.074	0.5894(15)
			0.122	0.3195(14)
			0.118	0.3440(16)
			0.088	0.5195(48)
			0.076	0.5898(81)

source-sink combinations, where the smearing is applied to the heavy quark. We compute the two- and three-point functions at several values of κ spanning a range from around the charm quark to the bottom quark. We determine $Z_{V_{\bar{q}q}^4}$ from a fit to the plateaus in the jackknifed ratio of the three-point and two-point functions. Our results are summarized in Table X.

In order to properly normalize the derivative $d\phi/d\kappa_Q$ [see Eq. (3.5)], we need values of $Z_{V_{\bar{q}q}^4}$ at κ values other than those used in the $Z_{V_{\bar{q}q}^4}$ simulations. We therefore fit the simulation results to the interpolating quartic polynomial

$$Z_{V_{\bar{q}q}^4}(\kappa) = 1 + \sum_{j=1}^4 c_j \kappa^j \quad (5.9)$$

which reproduces the infinite mass limit $Z_{V_{\bar{q}q}^4} \rightarrow 1$. Our codes employ the hopping-parameter version of the action; so, at tree level $c_1 = -6u_0$, and for $j > 1$, $c_j = 0$. We constrain the interpolation parameters to the tree-level values, taking $\sigma_j = 4$ as the widths. Table XI shows values for $Z_{V_{\bar{q}q}^4}$ interpolated to the nominal charm and

TABLE XI. Heavy-heavy vector current renormalization factor $Z_{V_{\bar{q}q}^4}$ corresponding to the charm and bottom κ_{sim} values used in the decay-constant simulations.

$\approx a$ [fm]	Charm		Bottom	
	κ_Q	$Z_{V_{\bar{q}q}^4}$	κ_Q	$Z_{V_{\bar{q}q}^4}$
0.09	0.127	0.2829(4)	0.0923	0.4891(9)
0.12	0.122	0.3029(4)	0.086	0.5216(10)
0.15	0.122	0.3199(14)	0.076	0.5868(81)

bottom κ_{sim} used in our decay-constant runs. Figure 2 plots the data in Table X together with the interpolation of Eq. (5.9). To aid perturbative intuition, the values of $Z_{V_{\bar{q}q}^4}$ in the figure are scaled by the tree-level expression $1 - 6u_0\kappa$; the relation between κ and $m_0 a/(1 + m_0 a)$ can be inferred from Eq. (4.4).

VI. CHIRAL AND CONTINUUM EXTRAPOLATION

In this section, we present the combined chiral and continuum extrapolations used to obtain the physical values of the $B_{(s)}$ and $D_{(s)}$ meson decay constants. We first discuss the use of $SU(3)$ chiral perturbation theory for heavy-light mesons in Sec. VIA, giving the formulas used for the chiral fits and describing our method for incorporating heavy-quark and light-quark discretization effects into the extrapolation. We then show the chiral fits for the D system in Sec. VIB, and for the B system in Sec. VIC.

A. Chiral perturbation theory framework

The errors introduced by the chiral and (light-quark) continuum extrapolations are controlled with rooted staggered chiral perturbation theory (r $S\chi$ PT) [25,26] applied to heavy-light mesons. In Ref. [42], the heavy-light decay constant was calculated to one loop in r $S\chi$ PT at leading order in the heavy-quark expansion $[(1/M_H)^0]$, where M_H is a generic heavy-light-meson mass. A replica trick is used in r $S\chi$ PT to take into account the effect of the fourth root of the staggered determinant [18,24].

In addition to using the form calculated in Ref. [42], we also use a chiral fit form that includes, in the loops, the effects of hyperfine splittings (e.g., $M_B^* - M_B$) and flavor splittings (e.g., $M_{B_s} - M_B$). These splittings are ~ 100 MeV, and so not much smaller than M_π , despite the fact that they are formally of order $1/M_H$. Since the lightest pseudoscalar meson masses in our simulations are ~ 225 MeV, it is not immediately obvious that including the splittings is necessary or useful. Their inclusion is motivated, first of all, by the observation of Arndt and Lin [82] that finite-volume effects in the one-loop diagrams can be substantially larger with the splittings present. This is mainly due to the fact that accidental cancellations in finite-volume effects between different diagrams at $(1/M_H)^0$ disappear once splittings are included. As described below, it is not difficult to include the splitting effects into the calculation of Ref. [42]. We also discuss the extent to which including the splittings, but not other effects that could occur at order $1/M_H$, is a systematic approximation. In practice, we do fits both including and omitting the splittings, and use the difference as one estimate of the chiral extrapolation error. For central values, we include the splittings, because this yields a more conservative estimate of finite-volume effects.

With staggered quarks, the (squared) pseudoscalar meson masses are

$$M_{ab,\xi}^2 = B_0(m_a + m_b) + a^2\Delta_\xi, \quad (6.1)$$

where m_a and m_b are quark masses, B_0 is a parameter of χ PT, and the representation of the meson under the taste symmetry group is labeled by $\xi = P, A, T, V, I$ [25]. The exact nonsinglet chiral symmetry of staggered quarks as $m_a, m_b \rightarrow 0$ ensures that $\Delta_P = 0$. All of these pseudoscalars appear in the “pion” cloud around the heavy-light meson in the simulation, and all of them therefore affect the decay constant.

Working at leading order $[(1/M_H)^0]$ in the heavy-quark expansion and at one loop, or next-to-leading order (NLO), in the chiral expansion, the $rS\chi$ PT expression for the decay constant with light valence quark q takes the form [42]

$$\begin{aligned} \phi_{H_q} = & \phi_H^0 \left[1 + \frac{1}{16\pi^2 f^2} \frac{1 + 3g_\pi^2}{2} \left\{ -\frac{1}{16} \sum_{e,\xi} \ell(M_{eq,\xi}^2) \right. \right. \\ & - \frac{1}{3} \sum_{j \in \mathcal{M}_I^{(2,q)}} \frac{\partial}{\partial M_{Q,I}^2} [R_j^{[2,2]}(\mathcal{M}_I^{(2,q)}; \mu_I^{(2)}) \ell(M_j^2)] \\ & - \left(a^2 \delta'_V \sum_{j \in \hat{\mathcal{M}}_V^{(3,q)}} \frac{\partial}{\partial M_{Q,V}^2} [R_j^{[3,2]}(\hat{\mathcal{M}}_V^{(3,q)}; \mu_V^{(2)}) \ell(M_j^2)] \right. \\ & \left. \left. + [V \rightarrow A] \right) \right] + p(m_q, m_l, m_h, a^2) \Big], \quad (6.2) \end{aligned}$$

where m_q is the light valence-quark mass and e runs over the sea quarks, the lighter two of which have masses m_l , and the heavier, m_h .² The parameter ϕ_H^0 is independent of the light masses, and p is an analytic function. We fit the charm and bottom systems separately, so ϕ_H^0 depends, in practice, on the heavy-quark mass. The meson mass $M_{Q,\xi}$ is similar to $M_{ab,\xi}$ in Eq. (6.1), but constructed from a valence quark-antiquark, $q\bar{q}$. The light-meson decay constant $f \approx f_\pi \cong 130.4$ MeV, and the $H-H^*-\pi$ coupling g_π controls the size of the one-loop effects. Taste-violating hairpin diagrams, which arise only at nonzero lattice spacing, are parametrized by δ'_A and δ'_V . The residue functions $R_j^{[n,k]}(\{M\}, \{\mu\})$ are defined in Ref. [26]. Chiral logarithms are written in terms of the functions $\ell(M^2)$ [83]:

$$\ell(M^2) = M^2 \ln \frac{M^2}{\Lambda_\chi^2} \quad [\text{infinite volume}], \quad (6.3)$$

$$\ell(M^2) = M^2 \left(\ln \frac{M^2}{\Lambda_\chi^2} + \delta_1(ML) \right) \quad [\text{spatial volume } L^3], \quad (6.4)$$

²The physical values of the average up-down quark mass and of the strange-quark mass are denoted by $\hat{m} = (m_u + m_d)/2$ and m_s , respectively.

$$\delta_1(ML) \equiv \frac{4}{ML} \sum_{r \neq 0} \frac{K_1(|r|ML)}{|r|}. \quad (6.5)$$

Here Λ_χ is the chiral scale, K_1 the Bessel function of an imaginary argument, and r any nonzero three-vector with integer components. The mass sets in the residue functions of Eq. (6.2) are

$$\mu^{(2)} = \{M_U^2, M_S^2\}, \quad (6.6)$$

$$\mathcal{M}^{(2,q)} = \{M_Q^2, M_\eta^2\}, \quad (6.7)$$

$$\hat{\mathcal{M}}^{(3,q)} = \{M_Q^2, M_\eta^2, M_{\eta'}^2\}, \quad (6.8)$$

where M_U (M_S) is the mass of the pseudoscalar $l\bar{l}$ ($h\bar{h}$) meson.

The salient feature of the chiral extrapolation of ϕ_{H_q} is that the chiral logs have a characteristic curvature as $m_q \rightarrow 0$ [84]. At nonzero lattice spacing, the presence of the additive splittings $a^2\Delta_\xi$ in the meson masses reduces the curvature of the chiral logarithms. The characteristic curvature returns, however, as the continuum limit is approached.

To combine data from several lattice spacings into one chiral extrapolation, it is necessary to convert lattice units to (some sort of) physical units. As mentioned in Sec. III A, we convert in two steps, first by canceling lattice units with the appropriate power of r_1/a . In particular, pseudoscalar meson masses [cf. Eq. (6.1)] become $r_1^2 M_{ab,\xi}^2 = (r_1/a)^2 \times (aM_{ab,\xi})^2$, and the decay constant [cf. Eq. (6.2)] becomes $r_1^{3/2} \phi_H = (r_1/a)^{3/2} (a^{3/2} \phi_H)$, with $a^{3/2} \phi_H$ determined from analyses I or II (cf. Sec. IV). Strictly speaking, one must take the quark-mass dependence of r_1 into account, either separately or by modifying the right-hand side of Eq. (6.2) accordingly. At the present level of accuracy, we ignore this subtlety, canceling units ensemble by ensemble with the computed r_1/a . Since r_1 is expected to depend smoothly on m_l and m_h , we are unlikely to introduce an uncontrolled error into the extrapolated decay constants. [After completing the chiral-continuum extrapolation in r_1 units, we then use $r_1 = 0.3117(22)$ fm (cf. Sec. III A) to convert to MeV.]

To quantify the size of NLO (and higher) corrections to χ PT, it is useful to define dimensionless parameters x_q, x_l , and x_h proportional to the quark masses m_q, m_l , and m_h :

$$x_{q,l,h} \equiv \frac{(r_1 B_0)(r_1/a)(2am_{q,l,h})}{8\pi^2 f_\pi^2 r_1^2}.$$

Since the splittings $a^2\Delta_\xi$ are added to the quark-mass terms in Eq. (6.1), it is similarly useful to define

$$x_{\Delta_\xi} \equiv \frac{r_1^2 a^2 \Delta_\xi}{8\pi^2 f_\pi^2 r_1^2}, \quad (6.9)$$

$$x_{\bar{\Delta}} \equiv \frac{r_1^2 a^2 \bar{\Delta}}{8\pi^2 f_\pi^2 r_1^2}, \quad (6.10)$$

where $\bar{\Delta}$ is the average pion splitting,

$$\bar{\Delta} = \frac{1}{16}(\Delta_P + 4\Delta_A + 6\Delta_T + 4\Delta_V + \Delta_I). \quad (6.11)$$

The x_i are in “natural” units for χ PT, in the sense that one expects that chiral corrections, when written as a series in the x_i , have coefficients [or low-energy constants (LECs)] that are of order 1.

We then take the analytic function p in Eq. (6.2) to have the following form at NLO:

$$L_{\text{val}}(x_q + x_{\Delta_{\text{val}}}) + L_{\text{sea}}(2x_l + x_h + 3x_{\Delta_{\text{sea}}}) + L_a \frac{a^2}{16\pi^2 f_\pi^2 r_1^4}, \quad (6.12)$$

where L_{val} , L_{sea} , and L_a are quark-mass-independent LECs that we fit from our data, and we define

$$x_{\Delta_{\text{val}}} \equiv \frac{9}{5}x_{\bar{\Delta}} - \frac{4}{5}x_{\Delta_I}, \quad (6.13)$$

$$x_{\Delta_{\text{sea}}} \equiv \frac{9}{11}x_{\bar{\Delta}} + \frac{2}{11}x_{\Delta_I}. \quad (6.14)$$

The low-energy constants L_{val} , L_{sea} , and L_a depend implicitly on the chiral scale Λ_χ , so that the complete expression, Eq. (6.2), is independent of Λ_χ . As in Ref. [42], we choose to include the a^2 -dependent terms $x_{\Delta_{\text{sea}}}$ and $x_{\Delta_{\text{val}}}$ in the coefficients of L_{val} and L_{sea} so that these coefficients represent those combinations of meson masses that arise naturally under a change of Λ_χ in the chiral logarithms.

The LEC L_a arises from analytic taste-violating effects; it serves as a counterterm to absorb changes proportional to the taste-violating hairpins δ'_A and δ'_V under a change in chiral scale. As such, we take the a^2 coefficient of L_a in Eq. (6.12) to vary with lattice spacing like $x_{\Delta_{\text{val}}}$. As long as L_a then appears as an independent fit parameter, the introduction of the $x_{\Delta_{\text{sea}}}$ and $x_{\Delta_{\text{val}}}$ terms in the coefficients of L_{val} and L_{sea} in Eq. (6.12) has a negligible effect on the results from the chiral fits. However, we find that the introduction of these terms significantly reduces the magnitude of L_a ; in other words, most of the discretization error from the light quarks appears to be due to the a^2 dependence of the light-meson masses in the chiral loops. We leave L_{val} , L_{sea} , and L_a unconstrained in the fits that determine central values; their size is of $O(1)$ as expected (and is in fact ≤ 0.6).

In the region of the strange-quark mass, the data for the decay constants show some curvature, and at least some quadratic terms in the quark masses (NNLO effects) must, in general, be added in order to obtain acceptable ($p > 0.01$) fits. There are four such LECs, giving a NNLO contribution to p of the form

$$Q_1 x_q^2 + Q_2 (2x_l + x_h)^2 + Q_3 x_q (2x_l + x_h) + Q_4 (2x_l^2 + x_h^2). \quad (6.15)$$

Fits omitting the Q_1 and Q_3 terms give poor confidence levels and are rejected; adding the Q_2 and Q_4 terms does not change the fit results much, but increases overall errors by up to 30%. To be conservative, we include all four terms in fits for central values; other acceptable fits (for example, fixing Q_2 or Q_4 or both to zero) are included among the alternatives used to estimate the systematic error of the chiral extrapolation.

For the central-value fits, the Q_i are mildly constrained by Gaussian priors with central value 0 and width 0.5, since that is roughly the expected size in natural units. After fitting, the posterior values satisfy $|Q_i| \leq 0.5$, and Q_1 and Q_3 have errors ≈ 0.05 (much less than the prior width), indicating that they are constrained by the data. Q_2 and Q_4 have errors ~ 0.5 , indicating that they are largely constrained by the priors. Changing the prior widths for the Q_i to 1.0 has a negligible effect on central values and errors of the decay constants, although the posterior Q_2 and Q_4 typically increase in size and error, as expected.

While the chiral form introduced so far gives acceptable simultaneous fits to our data from all available lattice spacings, we still need to estimate the size of heavy-quark and generic light-quark discretization errors. Following the Bayesian approach advocated in Refs. [71,72], we add constrained lattice-spacing-dependent terms to the fit function until the statistical errors of the results cease to increase appreciably. For the heavy quark, we take up to six such terms, $f_E(m_0 a)$, $f_X(m_0 a)$, $f_Y(m_0 a)$, $f_B(m_0 a)$, $f_3(m_0 a)$, and $f_2(m_0 a)$, where m_0 is the heavy-quark bare mass. Details about the origin and form of these six functions are given in Appendix A. These functions estimate fractional (not absolute) errors, and as such are included within the square brackets in Eq. (6.2) [or its equivalent, Eq. (6.20) below]. The first three are $O(a^2)$ corrections and are added to the fit with coefficients $z_i(a\Lambda)^2$, $i \in \{E, X, Y\}$, where Λ is a scale characteristic of the heavy-quark

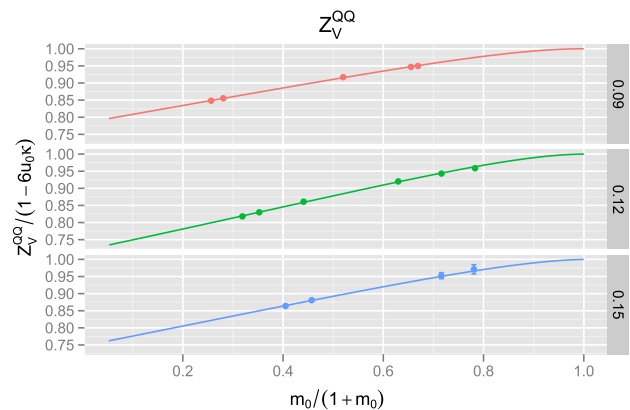


FIG. 2 (color online). Plot of $Z_V^{Q0}/(1 - 6u_0\kappa)$ vs $m_0/(1 + m_0 a)$ for the three lattice spacings.

expansion, and the z_i are parameters with prior value 0 and prior width 1 (for f_Y) or $\sqrt{2}$ (for f_E and f_X , since they each appear twice in the analysis of Appendix A). The next two terms are $O(\alpha_s a)$ corrections, added with coefficients $z_i \alpha_s a \Lambda$, $i \in \{B, 3\}$, with z_i taken to have prior value 0 and prior width 1 (for f_B) or $\sqrt{2}$ (for f_3 , again because it appears twice). The final term arises from the propagation to the decay constants of heavy-quark errors in the tuning of the heavy-quark hopping parameter, κ . It comes in with coefficient $z_2 (a\Lambda)^3$, with z_2 having prior value 0 and prior width 1. We take a large value $\Lambda = 700$ MeV, which provides conservatively wide priors, especially for the first five terms. Once one of each of the first two types of terms is added, the errors already reach $\sim 80\%$ of their values with all six added.

Similar terms representing generic light-quark errors, which are not automatically included in the fit function (unlike taste-violating terms), may also be added. With the Asqtad staggered action, generic discretization effects are of $O(\alpha_s a^2)$. We allow the physical LECs ϕ_H^0 , L_{val} , L_{sea} , Q_1 , Q_2 , Q_3 , and Q_4 to have small relative variations with lattice spacing with coefficients $C_i \alpha_s (a\Lambda)^2$, where i stands for any of the seven physical LECs, Λ is again taken to be 700 MeV, and the C_i have prior value 0 with prior width 1. This corresponds to a maximum of about a 3% difference for a given LEC between the $a \approx 0.12$ fm and the $a \approx 0.09$ fm ensembles. Once several heavy-quark discretization terms have been introduced, these light-quark terms further increase the total error of individual decay constants by less than 10%. However, the errors on the decay-constant ratios f_{D_s}/f_{D^+} and f_{B_s}/f_{B^+} are significantly increased by light-quark discretization effects, because the heavy-quark effects on the ratios cancel to the first approximation. For our central values, we include all six heavy-quark and all seven light-quark terms, so the total error from a given fit should estimate all (taste-conserving) discretization errors, as well as normal statistical effects. To estimate “heavy-quark” and “light-quark” discretization effects separately, we set to zero the light- or heavy-quark discretization terms, respectively, and then subtract the statistical errors in quadrature. Such separate errors are not relevant to any final results quoted below, but are included as separate lines in the error budget for informational purposes.

As mentioned above, our preferred fit form modifies Eq. (6.2) by including the effects of hyperfine and flavor splittings of the heavy-light mesons in one-loop diagrams. We now briefly describe how one may adjust the results of Ref. [42] to include these splittings. In Eq. (6.2), the contributions proportional to g_π^2 come from diagrams with internal H^* propagators, namely, the left-hand diagrams in Fig. 5 of Ref. [42]. Contributions with no factor of g_π^2 come from diagrams with light-meson tadpoles, namely, the right-hand diagrams in Fig. 5 of Ref. [42]. The latter have no internal heavy-light propagators, so are

unaffected by any heavy-light splittings. The splittings in the former diagrams depend on whether the light-meson line is connected (Fig. 5a, left, of Ref. [42]) or disconnected (Fig. 5b, left). In the disconnected case, the H^* in the loop always has the same flavor (q) as the external H_q , so there is no flavor splitting between the two, only a hyperfine splitting. In the connected case, the H^* in the loop has the flavor of the virtual sea-quark loop [which we labeled by e in Eq. (6.2)], so there is flavor splitting with the external H_q , in addition to the hyperfine splitting.

Let Δ^* be the (lowest-order) hyperfine splitting, and δ_{eq} be the flavor splitting between a heavy-light meson with light quark of flavor e and one of flavor q . At lowest order, δ_{eq} is proportional to the quark-mass difference (or light-meson squared mass difference), which can be written in terms of a parameter λ_1 :

$$\delta_{eq} \cong 2\lambda_1 B_0 (m_e - m_q) \cong \lambda_1 (M_E^2 - M_Q^2), \quad (6.16)$$

where M_E is the mass of an $e\bar{e}$ light meson. Here we have used the notation of Arndt and Lin [82] and included a factor of B_0 in the middle expression; B_0 is omitted in the notation of Ref. [85], Eq. (16), and of Ref. [42], Eq. (45).

By convention, the mass of the external H is removed in the heavy-quark effective theory, so the mass shell is at $k = 0$, where k is the external three-momentum. When there is no splitting, the internal H^* has its pole at the same place, which makes the integrals particularly simple, giving the chiral-log function $\ell(M^2)$, Eq. (6.3). If a splitting Δ is present, the integrals involve a significantly more complicated function, which we denote

$$J(M, \Delta) = (M^2 - 2\Delta^2) \log(M^2/\Lambda^2) + 2\Delta^2 - 4\Delta^2 F(M/\Delta) \quad [\text{infinite volume}], \quad (6.17)$$

Here the function F is most simply expressed [86,87] as

$$F(1/x) = \begin{cases} -\frac{\sqrt{1-x^2}}{x} \left[\frac{\pi}{2} - \tan^{-1} \frac{x}{\sqrt{1-x^2}} \right] & \text{if } |x| \leq 1 \\ \frac{\sqrt{x^2-1}}{x} \ln(x + \sqrt{x^2-1}) & \text{if } |x| \geq 1, \end{cases} \quad (6.18)$$

which is valid for all x .

It is then straightforward to write down the generalization of Eq. (6.2) to include splittings. The basic rule is to replace

$$\ell(M^2) \rightarrow J(M, \Delta) \quad (6.19)$$

in the terms proportional to g_π^2 . It is not hard to show that $J(M, 0) = \ell(M^2)$, so this replacement is consistent with the original result neglecting the splittings. In making the replacements, one must choose the correct value of the splitting Δ in each term. As mentioned above, in terms that come from the diagram with a disconnected light-meson propagator, one must put $\Delta = \Delta^*$. But in terms that come from the diagram with a connected light-meson propagator, one must put $\Delta = \Delta^* + \delta_{eq}$, because the

internal heavy-light meson is an H_e^* , while the external meson is an H_q . The result for the heavy-light-meson decay amplitude including the splittings is then

$$\begin{aligned} \phi_{H_q} = \phi_H^0 & \left[1 + \frac{1}{16\pi^2 f^2} \frac{1}{2} \left\{ -\frac{1}{16} \sum_{e,\Xi} \ell(M_{eq,\Xi}^2) - \frac{1}{3} \sum_{j \in \mathcal{M}_I^{(2,x)}} \frac{\partial}{\partial M_{X,I}^2} [R_j^{[2,2]}(\mathcal{M}_I^{(2,x)}; \mu_I^{(2)}) \ell(M_j^2)] \right. \right. \\ & - \left(a^2 \delta'_V \sum_{j \in \hat{\mathcal{M}}_V^{(3,x)}} \frac{\partial}{\partial M_{X,V}^2} [R_j^{[3,2]}(\hat{\mathcal{M}}_V^{(3,x)}; \mu_V^{(2)}) \ell(M_j^2)] + [V \rightarrow A] \right) \\ & - 3g_\pi^2 \frac{1}{16} \sum_{e,\Xi} J(M_{eq,\Xi}, \Delta^* + \delta_{eq}) - g_\pi^2 \sum_{j \in \mathcal{M}_I^{(2,x)}} \frac{\partial}{\partial M_{X,I}^2} [R_j^{[2,2]}(\mathcal{M}_I^{(2,x)}; \mu_I^{(2)}) J(M_j, \Delta^*)] \\ & \left. \left. - 3g_\pi^2 \left(a^2 \delta'_V \sum_{j \in \hat{\mathcal{M}}_V^{(3,x)}} \frac{\partial}{\partial M_{X,V}^2} [R_j^{[3,2]}(\hat{\mathcal{M}}_V^{(3,x)}; \mu_V^{(2)}) J(M_j, \Delta^*)] + [V \rightarrow A] \right) \right\} + p(m_q, m_l, m_h, a^2) \right]. \quad (6.20) \end{aligned}$$

It is also straightforward to include finite-volume effects into Eq. (6.20). One simply replaces

$$J(M, \Delta) \rightarrow J(M, \Delta) + \delta J(M, \Delta, L), \quad (6.21)$$

where $\delta J(M, \Delta, L)$ is the finite-volume correction in a spatial volume L^3 . The correction can be written in terms of functions defined in Refs. [44,82]:

$$\begin{aligned} \delta J(M, \Delta, L) = \frac{M^2}{3} \delta_1(ML) - 16\pi^2 & \left[\frac{2\Delta}{3} J_{\text{FV}}(M, \Delta, L) \right. \\ & \left. + \frac{\Delta^2 - M^2}{3} K_{\text{FV}}(M, \Delta, L) \right], \quad (6.22) \end{aligned}$$

with

$$K_{\text{FV}}(M, \Delta, L) \equiv \frac{\partial}{\partial \Delta} J_{\text{FV}}(M, \Delta, L), \quad (6.23)$$

and $\delta_1(ML)$ as given in Eq. (6.5).

Before turning to the fit details and results, we briefly discuss the extent to which including the splittings as in Eq. (6.20), and not other possible $1/M_H$ effects, is a systematic improvement on Eq. (6.2). In fact, in a parametric sense within the power counting introduced by Boyd and Grinstein [85], this is a systematic improvement, as long as we make some further specifications as to how Eq. (6.20) should be applied. As we detail below, however, the power counting of Ref. [85] is only marginally applicable to our data. For that reason we ultimately fit to both Eqs. (6.20) and (6.2) and take the difference as one measure of the chiral extrapolation error.

For the following discussion, let Δ be a generic splitting (Δ^* or δ_{eq} or a linear combination of the two) and M be a generic light pseudoscalar mass. The power counting introduced in Ref. [85] takes

$$\frac{\Delta^2, \Delta M, M^2}{M_H} \ll \Delta \sim M. \quad (6.24)$$

For our data, treating Δ and M as the same size is not dangerous, even though Δ is significantly smaller than our

simulation M values—at worst, this means that we include some terms unnecessarily. The condition $M^2/M_H \ll \Delta$, which is necessary to drop other $1/M_H$ contributions as still higher order, is marginally valid, however. For the D system, $M_K^2/M_D \approx 130$ MeV, which is roughly of the same size as Δ^* and δ_{sd} . For the B system, $M_K^2/M_B \approx 47$ MeV, of the same size as Δ^* but somewhat less than δ_{sd} . For the purposes of the chiral extrapolation, however, what matters is the applicability of the power counting at the lowest simulated light-meson masses, not its applicability at M_K .³ For our lightest simulated pions with mass $\sim M_K/2$, we can reduce the left side of the inequality in Eq. (6.24) by a factor of 4, at which point it becomes reasonably applicable.

Having tentatively accepted the power counting of Eq. (6.24), it is clear that $F(M/\Delta)$ in Eq. (6.17) should be treated as $\mathcal{O}(1)$. Then the difference between $J(M, \Delta)$ and the chiral logarithm it replaces, $\ell(M^2)$, is of the same order as $\ell(M^2)$ itself, so including the splittings becomes mandatory at the one-loop order to which we are working. The next question is whether Eq. (6.2) includes *all* effects to this order. As discussed by Boyd and Grinstein, the key issue is whether operators with two or more derivatives (two or more powers of residual momentum k) on the heavy fields can contribute. Such operators are suppressed by $1/M_H$ relative to the leading-order heavy-light Lagrangian, which has a single derivative. Since we are keeping Δ^* , which is also, in principle, a $1/M_H$ effect, one might worry that such operators could contribute at the same order. The power counting implies, however, that the relevant diagrams pick up a factor of $(\Delta, M)/M_H$ relative

³We assume here that the fit to the data is good over the full mass range simulated. It is not important for the chiral extrapolation that the fit be systematic in the region around M_K , but it must describe the data in that range so that we can correctly interpolate to the physical kaon mass. In Sec. VII, we check that the inclusion of points around M_K in the fit does not significantly affect the chiral extrapolation to light-quark mass.

to the terms being kept in Eq. (6.20). The reason for the difference is that the explicit extra factor of k turns into Δ or M —the only dimensional constants available—after integration. In the term that generates the hyperfine splitting itself, in contrast, the dimensional quantity balanced against $1/M_H$ is Λ —a heavy-quark QCD scale—rather than M . The power counting in Eq. (6.24) effectively treats Λ as larger than M (so that $\Delta \sim \Lambda^2/M_H \sim M$). Similarly, the term that generates the flavor splittings has a single factor of m_q and no residual momentum, and Eq. (6.24) effectively takes $m_q \sim k$ in such terms.

Boyd and Grinstein do find some other contributions at the same order as Eq. (6.20), but most come from terms that are simply Λ/M_H times terms in the leading-order heavy-light Lagrangian or current, and thus give simply an overall factor times the result without them. The exceptions are the terms multiplied by g_2 in Eq. (15) of Ref. [85] and by ρ_2 in Eq. (18) of Ref. [85]. These are operators that have the same dimension as the original Lagrangian current operators, but that violate heavy-quark spin symmetry, and therefore give different contributions to the pseudoscalar and vector meson decay constants at this order. Since we are only looking at pseudoscalar meson decay constants here, however, and since these effects are flavor independent, we can also absorb all of the $1/M_H$ effects into (1) the effects of the splittings in the loop, described by Eq. (6.20), and (2) an overall factor in front of the full one-loop result.

The overall factor in Eq. (6.20) is $1/(16\pi^2 f^2)$. Since f is not fixed at one loop, one should in any case allow it to vary over a reasonable range, which we take to be f_π to f_K . We allow such variations even when we fit to the form without splittings, Eq. (6.2). The difference between using f_π and f_K corresponds to a 45% change in the size of the one-loop coefficient, but produces only a 1 to 3 MeV change in the decay constants.⁴ We therefore assume that any further $1/M_H$ uncertainty in $1/(16\pi^2 f^2)$ has negligible effects on our results.

Finally, there is a question of whether terms coming from taste violations contribute something new at the same order in which we include splittings. Since taste-violating terms in the Lagrangian can enter just like light-quark masses, this is a possibility in principle. Corresponding to the terms in the quark masses that generate flavor splittings of heavy-light mesons [cf. Eq. (45) of Ref. [42]], there are taste-violating terms given in Eq. (51) of Ref. [42]. Just as for the quark-mass terms, however, we are only interested here in contributions that change the heavy-light-meson mass, not ones coupling the mesons to pion fields. When the pion fields are set to zero, all the terms in Eq. (51) of Ref. [42] just give a constant heavy-light-meson mass term proportional to a^2 that contributes

⁴Most of the change in the size of the overall coefficient is compensated by a change in the LECs that come from the fit to our data.

equally to the H and H^* masses of all valence flavors. Terms that produce a hyperfine splitting would have to also violate heavy-quark spin symmetry, and hence be of order $a^2\Lambda/M_H$. Similarly, terms that produce flavor splitting would need to violate flavor symmetry, and hence be of order $a^2 m_q/\Lambda_\chi$. Both such contributions are higher order in our power counting. Since there is no splitting, there is no contribution to the decay constants because the effect will vanish when we put the external B or D meson on mass shell.

In our chiral fits, we take the physical light-quark masses, as well as the parameters B_0 , $a^2\Delta_\xi$, δ'_A , and δ'_V , from the MILC Collaboration's results of rS χ PT fits to light pseudoscalar masses and decay constants [15,88] on ensembles that include lattice spacing $a \approx 0.15$ fm through $a \approx 0.06$ fm. Table XII shows the values used. In general, we use older MILC determinations since newer versions, e.g., those in Ref. [69], do not cover the full range of lattice spacings employed here (but are consistent where they overlap). The exceptions are the values of the taste-violating hairpin parameters $r_1^2 a^2 \delta'_A$ and $r_1^2 a^2 \delta'_V$. For them, the newer analysis including two-loop chiral logarithms gives larger systematic errors and a changed sign of the central value of $r_1^2 a^2 \delta'_V$, which has always been consistent with zero. For these parameters, we therefore use the wider ranges listed in Table XII, which encompasses both types of analyses. For comparison, the results of the analysis of Ref. [88] were $r_1^2 a^2 \delta'_A = -0.30(1)(4)$ and $r_1^2 a^2 \delta'_V = -0.05(2)(4)$.

In order to fit Eq. (6.20) to our lattice data, it is also necessary to input values for the hyperfine splitting Δ^* and for λ_1 in Eq. (6.16). For B mesons, we have [54]

$$\Delta^* = M_{B^*} - M_B \approx 45.8 \text{ MeV}, \quad (6.25)$$

$$\delta_{sd} = M_{B_s} - M_B \approx 87.0 \text{ MeV}, \quad (6.26)$$

$$\lambda_1 \approx 0.192 \text{ GeV}^{-1}, \quad (6.27)$$

where we use $M_E = M_S = 0.6858(40) \text{ GeV}$ [70] and $M_Q = M_{\pi^0} \approx 135.0 \text{ MeV}$ to obtain λ_1 from the experimental data. Similarly, for D mesons, we have

$$\Delta^* = M_{D_0^*} - M_{D_0} \approx 142.1 \text{ MeV}, \quad (6.28)$$

$$\delta_{sd} = M_{D_s} - M_{D_\pm} \approx 98.9 \text{ MeV}, \quad (6.29)$$

$$\lambda_1 \approx 0.219 \text{ GeV}^{-1}. \quad (6.30)$$

In the chiral fit, we input the relevant physical Δ^* and λ_1 from either Eqs. (6.26), (6.26), and (6.27) or (6.30), (6.29), and (6.30), and then use Eq. (6.16) with the actual m_c and m_q from each data point, and B_0 the slope for a given ensemble, from Table XII. We emphasize here that B_0 comes from a simple tree-level chiral fit of light-meson

TABLE XII. Inputs to our heavy-light chiral fits taken from the MILC Collaboration's light-meson chiral fits [15,88]. The physical bare-quark masses m_u , m_d , $\hat{m} \equiv (m_u + m_d)/2$, and m_s are determined by demanding that the charged pion and kaons take their physical masses after the removal of electromagnetic effects. Errors in the masses are due to statistics, chiral extrapolation systematics, scale determination, and (for m_d and m_u) the estimate of electromagnetic effects, respectively. "Continuum" values are found from chiral fits that have been extrapolated to the continuum, but masses are still in units of the "fine" ($a \approx 0.09$ fm) lattice spacing, and they would require the fine-lattice value of the mass renormalization constant to convert them to $\overline{\text{MS}}$ masses. Values for $r_1^2 a^2 \delta'_A$ and $r_1^2 a^2 \delta'_V$ take into account newer MILC analyses [69] as noted in the text. The light-meson analysis determining these quantities assumes that they scale like the taste-violating splittings Δ_ξ and are larger by a factor of 1.68 on the 0.15 fm lattices than on the 0.12 fm lattices, and smaller by a factor 0.35 on the 0.09 fm lattices than on the 0.12 fm lattices. The statistical and systematic errors on $r_1 B_0$ and $r_1^2 a^2 \Delta_\xi$ are not given here; such errors have a negligible effect on the heavy-light decay constants.

Quantity	Lattice spacing			
	$a \approx 0.15$ fm	$a \approx 0.12$ fm	$a \approx 0.09$ fm	"Continuum"
$am_s \times 10^2$	4.29(1)(8)(6)	3.46(1)(10)(5)	2.53(0)(6)(4)	2.72(1)(7)(4)
$a\hat{m} \times 10^3$	1.55(0)(3)(2)	1.25(0)(4)(2)	0.927(2)(27)(13)	0.997(2)(32)(14)
$am_d \times 10^3$	2.20(0)(4)(3)(5)	1.78(0)(6)(3)(4)	1.31(0)(4)(2)(3)	1.40(0)(5)(2)(3)
$am_u \times 10^4$	8.96(2)(17)(13)(49)	7.31(2)(23)(10)(40)	5.47(1)(16)(8)(30)	5.90(1)(19)(9)(32)
$r_1 B_0$	6.43	6.23	6.38	6.29
$r_1^2 a^2 \Delta_A$	0.351	0.205	0.0706	0
$r_1^2 a^2 \Delta_T$	0.555	0.327	0.115	0
$r_1^2 a^2 \Delta_V$	0.721	0.439	0.152	0
$r_1^2 a^2 \Delta_I$	0.897	0.537	0.206	0
$r_1^2 a^2 \delta'_A$	—	−0.28(6)	—	0
$r_1^2 a^2 \delta'_V$	—	0.00(7)	—	0

masses to Eq. (6.1). This is adequate for our purposes, since the resulting meson masses are only used within the one-loop chiral logarithms.

We can now present the actual chiral fits and show how we extract results and systematic errors from them. Recall that we compute ϕ_{H_q} for many combinations of the valence and light sea-quark masses, and at three lattice spacings: $a \approx 0.15$, 0.12 , and 0.09 fm. We fit all the decay-constant data to the form given either by Eq. (6.21) or by Eq. (6.4). One-loop finite-volume effects are included through Eq. (6.21) or Eq. (6.4). There are four unconstrained free parameters in our fits: the LO parameter ϕ_H^0 , and the one-loop LECs L_{val} , L_{sea} , L_a [Eq. (6.12)]. The central fit fixes the chiral coupling f at f_π , but a range of couplings are considered in alternative fits, as described in more detail in Sec. VII. Similarly, the H - H^* - π coupling g_π , which is poorly constrained by our data, is taken in the range 0.51 ± 0.20 . This encompasses a range of phenomenological and lattice determinations [86,89–94], as discussed in Ref. [56]. In the central fit, g_π is held fixed at 0.51, while it is varied in alternative fits described in Sec. VII. Although changing g_π is equivalent to changing f when splittings are omitted [cf. Eq. (6.2)], the effects are inequivalent when splittings are included [cf. Eq. (6.20)]. This is especially true of the finite-volume effects, for which the splittings have the potential to produce significant changes [82].

Some additional parameters constrained by Bayesian priors are also included in the chiral fits, as discussed above. The taste-violating hairpin parameters δ'_V and δ'_A are given by the ranges in Table XII. In addition, up to six heavy-quark and up to seven light-quark lattice-spacing-dependent terms are added for investigation of discretization effects. Except where otherwise noted, all 12 such terms are included in the fits plotted below: this gives errors that include true statistical errors plus our estimate of discretization effects from the heavy quarks and generic (taste nonviolating) discretization errors from the light quarks. In addition, some or all of the (mildly) constrained NNLO LECs, $Q_1, \dots, Q_4$, are included. Again, unless otherwise noted, the fits below include all four such parameters; such fits tend to give larger (and hence more conservative) errors than fits that restrict the number of these parameters. In total, there are 23 fit parameters in the central fits: the 19 constrained parameters listed in this paragraph, and the four unconstrained parameters listed in the previous paragraph.

B. Chiral fits and extrapolations for the D system

Figure 3 shows our central chiral fit to $r_1^{3/2} \phi_{D^+}$ and $r_1^{3/2} \phi_{D_s}$. Data from ensembles at $a \approx 0.15$ fm, $a \approx 0.12$ fm, and $a \approx 0.09$ fm are shown, but the $a \approx 0.15$ fm ensembles are not included in the fit. The points

and covariance matrix are obtained from analysis I (Sec. IV B) of the two-point functions. For clarity, only the unitary (full QCD) points are shown for ϕ_D (and approximately unitary for ϕ_{D_s}), but the fit is to all the partially quenched data on the $a \approx 0.12$ fm and $a \approx 0.09$ fm ensembles. The fit properly takes into account the covariance of the data; χ^2/dof and the p value (goodness of fit) are reasonable, as shown. The points in Fig. 3 are plotted as a function of mass m_x , where, for ϕ_{D^+} , the light valence mass m_q and the light sea mass m_l are given by $m_q = m_l = m_x$. For ϕ_{D_s} , only $m_l = m_x$ varies, while m_q is held fixed at the value m_{s_v} near the physical strange mass m_s .⁵ In order to be able to compare ensembles at different lattice spacings, we have adjusted the bare-quark masses by the ratio $Z_m/Z_m^{0.09 \text{ fm}}$, where Z_m is the (one-loop) mass renormalization constant [95], and $Z_m^{0.09 \text{ fm}}$ is its value on the $a \approx 0.09$ fm ensembles.

The continuum extrapolation is carried out by taking the fitted parameters and setting $a^2 = 0$ in all taste-violating terms (parametrized by Δ_ξ , δ'_A , δ'_V , and L_a), all heavy-quark discretization effects (parametrized by z_E , z_X , z_Y , z_B , z_3 , and z_2), and all generic light-quark discretization effects (parametrized by C_i). The red lines (solid for ϕ_{D^+} , dotted for ϕ_{D_s}) show the effect of extrapolating to the continuum and setting the strange-quark mass (both sea, m_h , and valence, m_{s_v}) to the physical value m_s .

Finally, the bursts give the result after the chiral extrapolation in the continuum, i.e., setting $m_x = m_d$ for ϕ_{D^+} and $m_x = \hat{m}$ for ϕ_{D_s} . The larger, dark red, error bars on the bursts show the total error from the fit, which includes heavy-quark and generic light-quark discretization errors using Bayesian priors, as described above. The smaller, bright red error bars show purely statistical errors, which are computed by a fit with all the discretization prior functions turned off. In plotting the red line for ϕ_{D^+} , the light sea mass is shifted slightly ($m_l = m_x + \hat{m} - m_d$) so that it takes its proper mass when $m_x = m_d$. (We neglect isospin violations in the sea.) The small mass differences between $\hat{m}$ and m_d (and the corresponding difference between $\hat{m}$ and m_u for the B^+) produce changes in ϕ that are much smaller than our current errors, but we include them here with an eye to future work, where the precision will improve.

The trend of the data for the coarsest lattice spacing ($a \approx 0.15$ fm, the magenta points in Fig. 3) tends to be rather different than for the finer lattice spacings, especially for the D_s , which is why we exclude the $a \approx 0.15$ fm data from the central fit. This trend is even more exagger-

⁵On the $a \approx 0.15$ fm ensembles, m_{s_v} is equal to the value of the strange sea quark mass m_h ($am_{s_v} = 0.0484$), but on the other two ensembles we take it lower than m_h , because m_h has been chosen somewhat larger than the physical strange mass. In the figure, $am_{s_v} = 0.415$ for the $a \approx 0.12$ fm ensembles and $am_{s_v} = 0.272$ for the $a \approx 0.09$ fm ensembles.

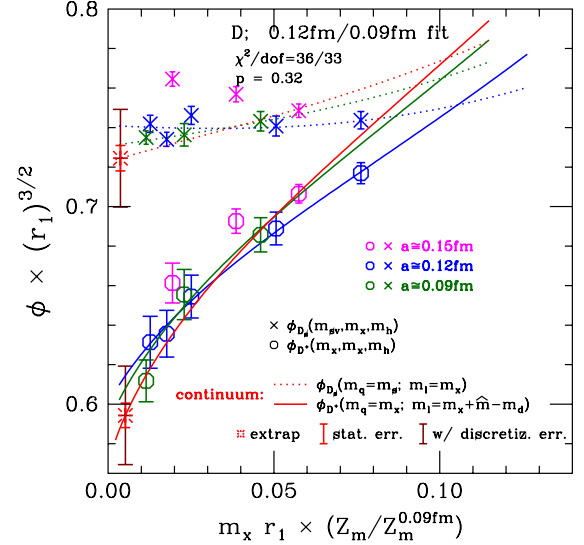


FIG. 3 (color online). Central chiral fit for the D system, based on analysis I of the fits to two-point correlators. Only (approximately) unitary points are shown. Data from ensembles at $a \approx 0.15$ fm, $a \approx 0.12$ fm, and $a \approx 0.09$ fm are shown, but the $a \approx 0.15$ fm ensembles are not included in the fit. The bursts show extrapolated values for ϕ_{D_s} and ϕ_{D^+} , with the purely statistical errors in bright red and the statistical plus discretization errors in darker red. The physical strange-quark mass corresponds to an abscissa value of $m_x \approx 0.1$.

ated for the B system, but with particularly large statistical errors; see Fig. 6 below. Nevertheless, the effect of including the $a \approx 0.15$ fm points in the fit is a rough indication of the size of discretization errors. Figure 4 shows what happens to the fit when these points are included: ϕ_{D^+} and ϕ_{D_s} each move up an amount comparable to (but less than) the size of the larger (dark red) error bars, which

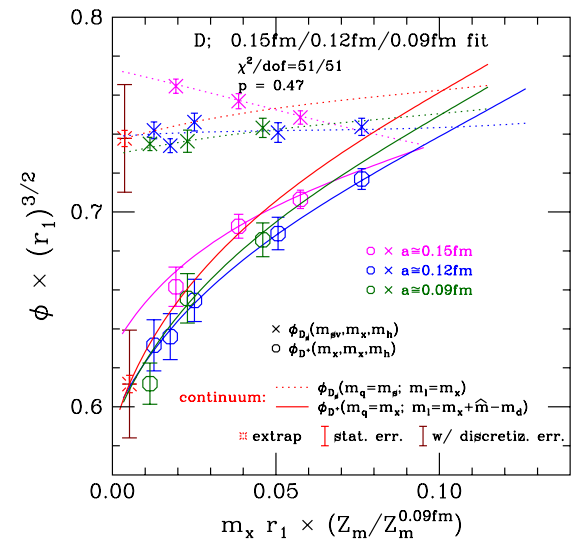


FIG. 4 (color online). Same as Fig. 3, but including points at $a \approx 0.15$ fm in the chiral-continuum fit.

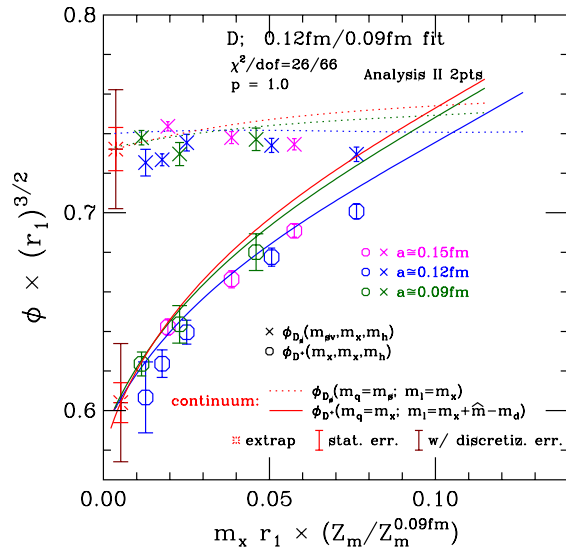


FIG. 5 (color online). Same as Fig. 3, but using analysis II of the two-point function.

represent heavy and generic light-quark discretization errors (as well as statistical errors, which are smaller). The consistency is reassuring.

As discussed in Sec. IV, we also examine analysis II of the two-point functions. Figure 5 shows the effect of using analysis II in the chiral fits. The differences in the decay-constant results between Figs. 3 and 5 are included in the decay-constant error budgets as a “fitting error.” Note that the covariance matrix calculation in analysis II results in an apparent underestimate of χ^2 (and, consequently, a high apparent p value). We believe that this stems from binning of the data to remove autocorrelation effects, which has the disadvantage of reducing the number of samples used to compute the covariance matrix. It is then difficult to determine small eigenvalues accurately. Indeed, the eigenvalues of the (normalized) correlation matrix tend to have a lower bound of $\sim 10^{-4}$ to 10^{-3} with this approach, whereas they typically go down to 10^{-5} in analysis I. [Recall that in analysis I we keep all samples, and deal with autocorrelation effects by Eq. (4.13).] Nevertheless, the difficulty with small eigenvalues explains only a small fraction of the difference between the results from analyses I and II. For example, f_D is changed by only 0.2 MeV when we smooth eigenvalues from analysis I that are less than 10^{-3} , following the method of Ref. [96]. This may be compared to the total difference between f_D in analyses I and II, which is 1.7 MeV.

C. Chiral fits and extrapolations for the B system

Results for the B system closely resemble those for the D system in most respects. One important difference is that the signal-to-noise ratio is worse for the B system because the mass difference that controls the noise, $2m_B - m_{\eta_b} - m_\pi$, increases with the mass of the heavy quark [97]. Therefore, the preferred fit in analysis I for the charm

case (large $t_{\min}$ with only the ground state and a single opposite-parity excited state) is too noisy here, and we must use fits with an extra excited state and smaller $t_{\min}$ (see Sec. IV B). Consequently, our B -system results have larger statistical errors. On the other hand, heavy-quark discretization errors are smaller in the B system. In the HQET analysis of discretization effects, they appear in the heavy-quark expansion, which works better for B ’s to begin with [63].

Figure 6 shows, for unitary points only, our central chiral fit for the B system. This is based on analysis I of the two-point functions. As in Fig. 3, the red lines (solid for ϕ_{B^+} , dotted for ϕ_{B_s}) show the effect of extrapolation to the continuum and setting the strange-quark mass to its physical value m_s . For the solid red line, the light sea mass is again shifted slightly, but now $m_l = m_x + \hat{m} - m_u$, so that it takes its proper mass when $m_x = m_u$. The bursts show the final results and come from setting $m_x = m_u$ for ϕ_{B^+} and $m_x = \hat{m}$ for ϕ_{B_s} . As before, the smaller, bright red, error bars show purely statistical errors, and the larger, dark red, error bars come from the fit with Bayesian priors and include heavy-quark and generic light-quark discretization errors as well as statistical errors.

In Fig. 6, the $a \approx 0.15$ fm data are both noisy and far from those of the finer lattice spacings. Therefore, these ensembles are again dropped from the central fit. Figure 7 shows the effect of including the $a \approx 0.15$ fm points. Note that the resulting continuum-extrapolated line for ϕ_{B_s} ,

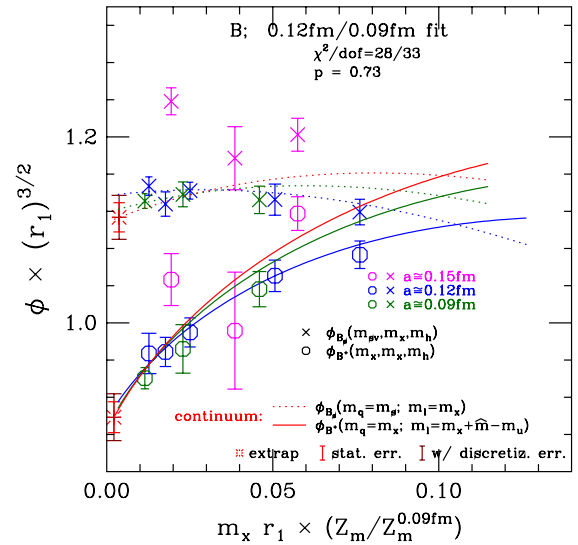


FIG. 6 (color online). Central chiral fit for the B system, with data from analysis I of the two-point functions. Only (approximately) unitary points are shown. Data from ensembles at $a \approx 0.15$ fm, $a \approx 0.12$ fm, and $a \approx 0.09$ fm are shown, but the $a \approx 0.15$ fm ensembles are not included in the fit. The bursts show extrapolated values for ϕ_{B_s} and ϕ_{B^+} , with the purely statistical errors in bright red and the statistical plus discretization errors in darker red. The physical strange-quark mass corresponds to an abscissa value of $m_x \approx 0.1$.

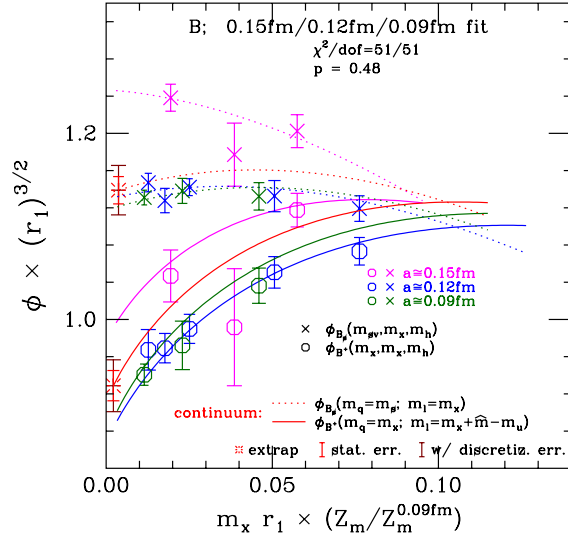


FIG. 7 (color online). Same as Fig. 6, but including points at $a \approx 0.15$ fm in the fit.

(dotted red line) now has what appears to be a rather unphysical shape, showing a significant initial increase as the light sea-quark mass is decreased, starting at the right side of the graph. There are several possible causes for the large discretization effects at $a \approx 0.15$ fm. These include heavy-quark effects (aM_H takes its largest value in our analysis, ~ 4 , on these points), light-quark taste violations ($a \approx 0.15$ fm ensembles are often excluded from light-quark analyses [98] because of large a^4 corrections), and the fact that the improved gauge action does not remove $O(\alpha_s a^2)$ errors due to quark loops. In addition, there is the simple problem of the large statistical noise for the B system, which is worst at the coarsest lattice spacing, as

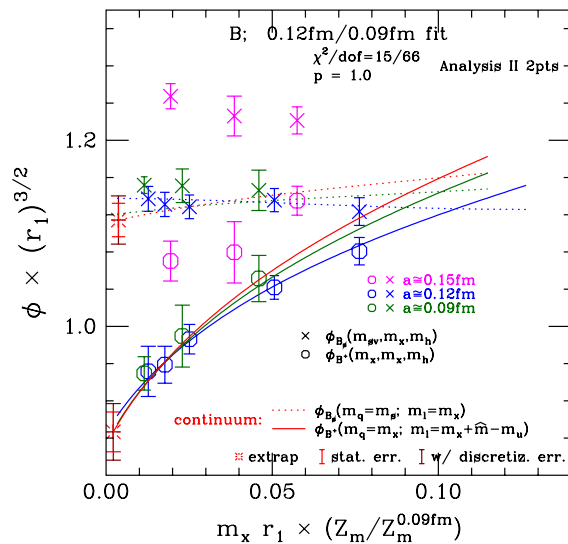


FIG. 8 (color online). Same as Fig. 6, but using analysis II of the two-point functions.

seen clearly in Fig. 7. The end result is that the differences caused by including the $a \approx 0.15$ fm points in the standard (Bayesian) fit are 10% to 20% larger than the dark red error bars in Fig. 6, and 40% to 60% larger than discretization errors estimated by removing the statistical errors from the dark red bars. Because the trend for $a \approx 0.15$ fm is so different from the other spacings, and because of the unphysical behavior when these points are included in the fit, we believe this difference overestimates the true discretization error. Nevertheless, to be conservative, we increase the discretization error estimate to take into account the effect of including the $a \approx 0.15$ fm ensembles, as described in Sec. VII.

Figure 8 shows the effect of using analysis II of the correlation functions. In order to make these comparisons as direct as possible, we first turn off all the Bayesian discretization terms in the fits. Compared to the results from Fig. 6, this fit gives a value of f_{B_s} about 1 MeV higher and a value of f_{B^+} about 2 MeV lower. These differences are included in our estimate of the fitting errors due to excited state contamination in Sec. VII.

VII. ESTIMATION OF SYSTEMATIC ERRORS

In this section, we present a careful, quantitative accounting for the uncertainties in our calculation. We consider, in turn, discretization errors, fitting errors, errors from inputs r_1 and quark-mass tuning, renormalization, and finite-volume effects. Table XIII details our error budget.

A. Heavy-quark and generic light-quark discretization effects

As described in Sec. VI and Appendix A, we parametrize possible heavy-quark and generic light-quark discretization effects and follow a Bayesian approach in including such effects in our chiral fitting function. Consequently, the raw “statistical” error that comes from our fits is not a pure statistical error but includes an estimate of the errors coming from the discretization effects. This inclusive error is shown with the dark red error bars in the plots in Sec. VI. For the D system, it is listed in the first line of Table XIII.

In the B system, the effect on the continuum-extrapolated results caused by including the $a \approx 0.15$ fm data can be somewhat larger than the discretization error estimated in the Bayesian approach. To be conservative, we therefore replace the Bayesian estimates in such cases with the difference between a fit with and without the $a \approx 0.15$ fm ensembles included. (These comparison fits do not themselves include the Bayesian discretization error terms.) The pure statistical error is then added in quadrature to the difference to get the “statistics $\oplus$ discretization” error shown for f_{B^+} and f_{B_s} in Table XIII. (For the ratio f_{B_s}/f_{B^+} , the Bayesian estimate was larger than the

TABLE XIII. Total error budget for the heavy-light decay constants. Uncertainties are in MeV for decay constants. The total combines errors in quadrature. The first row includes statistics, heavy-quark discretization errors, and generic light-quark discretization errors, as explained in the text. Errors in parentheses are approximate subparts of errors that are computed in combination.

Source	f_{D^+} (MeV)	f_{D_s} (MeV)	f_{D_s}/f_{D^+}	f_{B^+} (MeV)	f_{B_s} (MeV)	f_{B_s}/f_{B^+}
Statistics $\oplus$ discretization	9.2	8.9	0.014	5.8	6.0	0.013
(statistics)	(2.3)	(2.3)	(0.005)	(3.6)	(3.4)	(0.010)
(heavy-quark disc.)	(8.2)	(8.3)	(0.007)	(3.8)	(4.3)	(0.004)
(light-quark disc.)	(2.9)	(1.5)	(0.012)	(2.5)	(2.5)	(0.007)
Chiral extrapolation	3.2	2.2	0.014	2.9	2.8	0.014
Two-point functions	3.3	1.6	0.013	3.0	4.1	0.015
Scale (r_1)	1.0	1.0	0.001	1.0	1.4	0.001
Light-quark masses	0.3	1.4	0.005	0.1	1.3	0.006
Heavy-quark tuning	2.8	2.8	0.003	3.9	3.9	0.005
u_0 adjustment	1.8	2.0	0.001	2.5	2.8	0.001
Finite volume	0.6	0.0	0.003	0.5	0.1	0.003
$Z_{V_{00}^q}$ and $Z_{V_{qq}^q}$	2.8	3.4	0.000	2.6	3.1	0.000
Higher-order $\rho_{A_4}^{Qq}$	1.5	1.8	0.001	1.4	1.7	0.001
Total error	11.3	10.8	0.025	9.1	10.0	0.026

error determined this way, so we use the former.) For comparison, the Bayesian-determined errors for f_{B^+} and f_{B_s} are 5.5 and 5.1 MeV, respectively.

For informational purposes, it is useful to break down this inclusive error into its component parts, at least approximately. We can see what errors to expect and, hence, target for improvement in future simulations. In particular, with our current actions, the light-quark and heavy-quark discretization errors should behave differently as a function of lattice spacing, with heavy-quark errors decreasing more slowly as a is reduced. To extract the pure statistical errors, we rerun the fits with all the Bayesian discretization terms set to zero. We then find the pure heavy-quark (or pure light-quark) discretization contributions, by turning back on the heavy-quark (light-quark) terms, and then subtracting in quadrature the pure statistical errors from the resulting raw errors. These individual errors are shown in Table XIII in parentheses. Note that the total error at the bottom of the table includes the error on the first line, not the sum of the three errors in parentheses, when these differ. Note also that the discretization errors are similar to what we would have obtained with less sophisticated power counting.

B. Chiral extrapolation and taste-violating light-quark discretization effects

As described in Sec. VI, we modify the chiral fit function in a variety of ways to estimate the error associated with the chiral extrapolation.

- $\chi 1$. Set the chiral coupling f to f_K instead of f_π .
- $\chi 2$. Allow the chiral coupling f to be a Bayesian fit parameter, with prior value f_π and prior width equal to $f_K - f_\pi$.

$\chi 3$. Replace the $H-H^*-\pi$ coupling g_π (which is 0.51 in the central fit) with 0.31 or 0.71, which are the extremes of the range discussed in Sec. VI.

$\chi 4$. Allow g_π to be a constrained fit parameter, with prior value 0.51 and prior width 0.20.

$\chi 5$. Fix to zero those NNLO analytic terms [Q_2 and/or Q_4 in Eq. (6.15)] that may be eliminated without making the fit unacceptably poor.

$\chi 6$. Use the chiral function without hyperfine and flavor splittings, i.e., use Eq. (6.2) instead of Eq. (6.20).

$\chi 7$. Use combinations of modifications $\chi 1$ and $\chi 3$ or modifications $\chi 2$ and $\chi 3$. These choices can produce significantly larger deviations since changes in g_π have a similar effect on the fit function as changes in f .

These modifications typically change the decay constant by 1–3 MeV, and the ratios by 1%–1.5%. We take the chiral extrapolation error of a given quantity to be the largest change (of either sign) under the above modifications, and list it in Table XIII. In several cases (f_{D^+} , f_{D_s}/f_{D^+} , and f_{B_s}/f_{B^+}) the largest change comes from modification $\chi 6$, eliminating the heavy-light splittings. The fit without the splittings is shown for the D system in Fig. 9. It may be compared to Fig. 3 to see the effects: the curvature at small mass for ϕ_{D^+} is slightly greater without the splittings, which results in a decrease of f_{D^+} of 3.2 MeV. Note that the p values of the two fits are almost identical, so the goodness of fit cannot be used to choose one version of the chiral extrapolation over the other.

Modifications of f and/or g_π produce the largest changes in the other quantities, namely, f_{D_s} , f_{B^+} , and f_{B_s} . In particular, putting $f = f_K$ and $g_\pi = 0.31$ results in an increase of +2.9 for f_{B^+} and +2.8 MeV for f_{B_s} . The modified fit is shown in Fig. 10, and may be compared with Fig. 6 to see the effects of the changes. Increasing f and

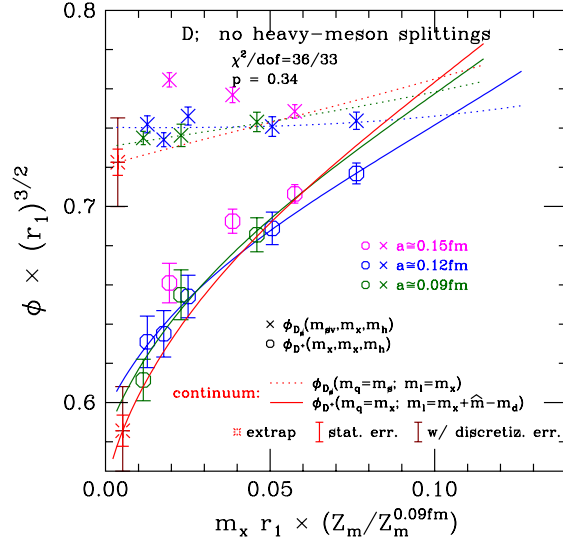


FIG. 9 (color online). Same as Fig. 3, but omitting heavy-light hyperfine and flavor splittings in the chiral fit function.

decreasing g_π both suppress the chiral logarithms [cf. Eq. (6.20)] and give fit functions with less curvature and smaller slope at low quark mass.

In Sec. VIA, we argued that the fact that the chiral power counting is at best marginally applicable in the neighborhood of M_K is not a problem for the chiral extrapolation. To test this, we remove the largest two valence-quark masses from each ensemble and repeat the analysis. The heaviest valence masses are then $0.73m_s$ on the $a \approx 0.09$ fm ensembles and $0.58m_s$ on the $a \approx 0.12$ fm ensembles. For all quantities, the differences in final results from the central analysis are comparable to or less than the purely statistical errors, and always significantly less than the chiral error determined by the comparisons $\chi^2_{1-\chi^2_7}$

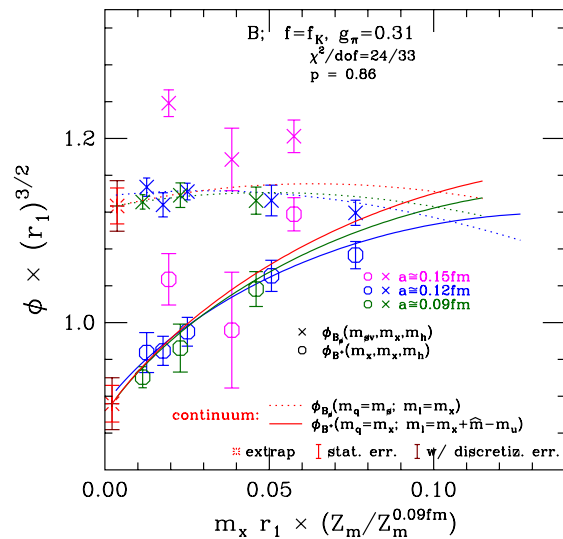


FIG. 10 (color online). Same as Fig. 6, but with $f = f_K$ and $g_\pi = 0.31$ in the chiral fit function.

above. Furthermore, the chiral fit parameters never change by more than the statistical errors.

Since the $rS\chi$ PT fit functions in Eqs. (6.2) and (6.20) explicitly include one-loop discretization effects coming from taste violations in the (rooted) staggered light-quark action, the chiral error estimates we describe here inherently include taste-violating discretization errors. However, it seems unlikely that the current data can accurately distinguish between such taste-violating errors of order $\alpha_s^2 a^2$ and generic light-quark discretization effects of order $\alpha_s a^2$, or even heavy-quark discretization effects. Indeed, the taste-violating LEC L_a [cf. Eq. (6.12)] is not well constrained by our fits and is consistent with zero within large errors. The central fits give

$$L_a = +0.6 \pm 6.5 \quad (D \text{ system}), \quad (7.1)$$

$$L_a = -1.9 \pm 8.8 \quad (B \text{ system}), \quad (7.2)$$

where the error is the raw statistical error. (Note that we do not constrain L_a by any prior width.) The errors in L_a decrease by about 10% if Bayesian parameters for generic light-quark errors are removed, and an additional 10% if the parameters for heavy-quark errors are removed. Thus, there is “cross talk” between various error sources, making it difficult to completely distinguish the various types of discretization errors. Future work, with more and finer lattice spacings, should make a cleaner separation possible.

C. Fitting errors

The “fitting errors” are the errors introduced in the analysis of the two-point correlators. They represent the effects of various choices of fit ranges and fitting functions and are an estimate of the systematic effect of the contamination by excited states. We compare results from the three choices of two-point fitting (see Sec. IV): analysis I, analysis II, and a modified analysis I using one simple + 1 oscillating state but values of $t_{\min}$ larger than those described in Sec. IV B.

Some of these differences may, in fact, be due simply to statistical effects, and hence already included in the statistical error. Figure 11 shows the differences between values of ϕ_{B_q} in analyses I and II, divided by the average statistical error for each of the common partially quenched data points. Only 10 of 74 differences are greater than one statistical σ . Nevertheless, there appears to be some significant systematic trend in that 46 of 74 points are positive. To be conservative, we take the largest difference between the analysis I fits and the other two fits as the fitting error for each physical quantity, and list it in Table XIII. For f_{D_s} and f_{B_s} , the difference is largest for chiral fits based on two-point analysis II, while, for the other four quantities, the difference is largest for the modified analysis I.

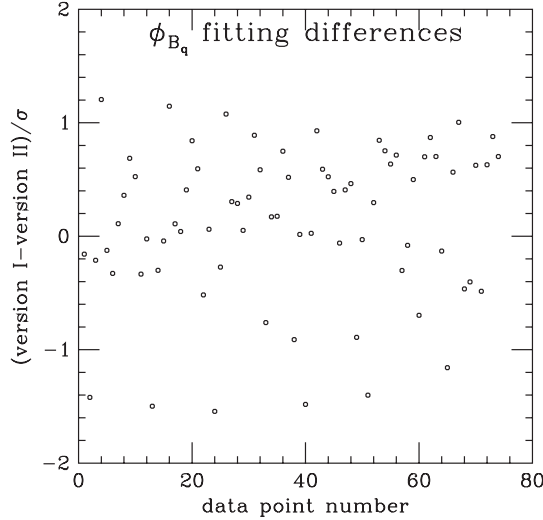


FIG. 11. Difference of ϕ_{B_q} values from analyses I and II, divided by the average statistical error at each of the common valence and sea mass points. The order along the abscissa is arbitrary.

D. Scale uncertainty

We use the scale $r_1 = 0.3117(22)$ fm to tune the values of the quark masses and convert the decay constants into physical units (see Sec. III A). To find the scale errors on the final results, we shift r_1 to 0.3139 fm or 0.3095 fm and redo the analysis. Although ϕ_H scales like $r_1^{-3/2}$, the change in the results under a change in r_1 is smaller than pure dimensional analysis would imply, because our estimates of the physical light masses and the heavy-quark κ_c and κ_b also shift, producing partially compensating changes in ϕ_H . At $r_1 = 0.3139$ fm, we shift the light masses in Table XII upward by the scale error shown in that table. [The lattice light-quark masses scale like r_1^2 , because they are approximately linear in the squared meson masses $(r_1 m_\pi)^2$ and $(r_1 m_K)^2$.] Similarly, we shift the tuned κ_c and κ_b downward by the scale error in Table V because the bare heavy-quark mass increases with r_1 . We then adjust $\phi_{B(s)}$ and $\phi_{D(s)}$ at each lattice spacing using Eq. (3.5) and the values of $d\phi/d\kappa$ given in Table V. Redoing the preferred chiral fits shown in Figs. 3 and 6, extrapolating to the continuum, and plugging in the adjusted continuum light-quark masses gives the scale error listed in Table XIII.

E. Light-quark-mass determinations

To estimate the error from the light-quark-mass determination, we follow a similar procedure to that in the scale-error case. We shift the continuum light-quark masses in Table XII by the sum in quadrature of all errors except scale errors. This includes the statistical errors, the chiral errors and, where relevant, the electromagnetic errors. We then plug the new masses into the continuum-extrapolated chiral fits and take the difference from the central results to

give the errors listed in Table XIII. The relative direction of shifts on different masses makes little difference in the size of the errors on the decay constants f_{D_s} , f_{D^+} , f_{B_s} , and f_{B^+} , since they are sensitive primarily to the valence-quark masses. However, it does affect the error of the ratios f_{D_s}/f_{D^+} and f_{B_s}/f_{B^+} . The largest effect clearly occurs when the strange mass is shifted in the opposite direction from the lighter masses. To be conservative, we take the size of change of the ratios in this case as the error, but this is almost certainly an overestimate because the statistical and chiral extrapolation errors on the light-quark masses are positively correlated between the strange mass and the other masses.

Note that the errors from the light-quark masses in Table XIII are much larger for f_{D_s} and f_{B_s} than for f_{D^+} and f_{B^+} . That simply reflects the facts that the decay constants have a nonzero limit when the quark masses vanish, and that the dependence on the quark masses is reasonably linear. Thus a given percent error in the strange mass produces a much larger percent difference in f_{D_s} and f_{B_s} than the same percent error in the d or u mass does in f_{D^+} and f_{B^+} .

F. Bottom- and charm-quark mass determinations

The propagation of statistical errors in the tuned κ_c and κ_b to the decay constants is complicated by the fact that the independent errors at each lattice spacing affect the final results in a nontrivial way through the continuum and chiral extrapolations. At each lattice spacing, we choose 200 Gaussian-distributed ensembles of trial κ values with central value equal to the tuned values and standard deviation equal to the statistical error, taken from Table V. For a given choice of trial κ values at each lattice spacing, we produce an adjusted trial data sample by shifting the ϕ_H values according to Eq. (3.5), but with the trial values replacing the tuned values. We then perform the complete chiral fit and extrapolation procedure on each of the 200 trial data sets. The standard deviation over trials of a given decay constant or decay-constant ratio is taken to be the heavy-quark tuning error, and is listed in Table XIII.

G. Tadpole factor (u_0) adjustment

In order to improve the convergence of lattice perturbation theory, we use tadpole-improved actions for the gluons, light quarks, and heavy quarks [79]. For the gluon and sea-quark actions we take the tadpole factor u_0 from the average plaquette. On the $a \approx 0.15$ fm and $a \approx 0.09$ fm lattices we use the same choice for the light valence and heavy-quark actions. On the $a \approx 0.12$ fm lattices, however, we use the tadpole factor u_0 taken from the Landau link in the valence-quark action and in the clover term in the heavy-quark action. This results in a slight mismatch between the light valence and sea-quark actions on these ensembles, and also affects the values obtained for the

tuned bottom- and charm-quark masses κ_b and κ_c . The difference between u_0 obtained from the average plaquette and the Landau link is approximately 3%–4% on the $a \approx 0.12$ fm ensembles.

We propagate this difference through the chiral/continuum extrapolation as follows. First, we compute the heavy-strange meson decay amplitudes ϕ_{B_s} and ϕ_{D_s} with both choices for u_0 on the ensemble with $am_l/am_h = 0.01/0.05$, $a \approx 0.12$ fm. For each choice of u_0 , we compute ϕ_{B_s} and ϕ_{D_s} directly at the tuned values of κ_b and κ_c , thereby avoiding an interpolation in κ . Next, we renormalize the lattice decay amplitudes using the nonperturbative, flavor-diagonal current renormalization factors $Z_{V_{qq}^4}$ and $Z_{V_{QQ}^4}$ obtained for each case. (We neglect the slight difference in the perturbative correction $\rho_{A_{Qq}^4}$.) Then, we calculate the ratio of the renormalized decay amplitudes, finding no difference within errors:

$$\phi_c^{\text{plaquette}}/\phi_c^{\text{Landau}} = 1.005(13), \quad (7.3)$$

$$\phi_b^{\text{plaquette}}/\phi_b^{\text{Landau}} = 1.014(20). \quad (7.4)$$

As expected, the u_0 dependence from the bare current and renormalization factors mostly cancels. Finally, we repeat the chiral/continuum extrapolation, shifting ϕ_c and ϕ_b on the $a \approx 0.12$ fm ensembles by the statistical errors reported in Eqs. (7.3) and (7.4). We find that these percent-level errors in ϕ_c and ϕ_b lead to approximately 1% errors in the extrapolated decay constants and approximately 0.1% errors in the decay-constant ratios. These errors are listed as “ u_0 adjustment” in the error budget in Table XIII.

H. Heavy-light current renormalization

There are two sources of systematic error in our heavy-light current renormalization. The first is due to the perturbative calculation of $\rho_{A_{Qq}^4}$, and the second is due to the nonperturbative calculation of $Z_{V_{qq}^4}$ and $Z_{V_{QQ}^4}$.

The perturbative calculation of $\rho_{A_{Qq}^4}$ has been carried out to one-loop order. Since $\rho_{A_{Qq}^4}$ is defined from a ratio of renormalization factors [see Eq. (2.5)], its perturbative corrections are small by construction. Indeed, as can be seen from the results for $\rho_{A_{Qq}^4}$ given in Table VIII, we observe very small corrections. For bottom they range from 0.3% at $a \approx 0.09$ fm to 0.8% at $a \approx 0.12$ fm and 2.8% at $a \approx 0.15$ fm. For charm they range from less than 0.08% at $a \approx 0.09$ fm to 0.4% at $a \approx 0.12$ fm and 0.6% at $a \approx 0.15$ fm. As shown in Ref. [46] the perturbative corrections to the ρ factors for the spatial currents, while still small, tend to be bigger than those for the temporal currents A^4 and V^4 . We therefore estimate the error due to neglecting higher-order terms as $\rho_{V_{Qq}^4}^{[1]} \alpha_s^2$. We take α_s at

$a \approx 0.09$ fm and $\rho_{V_{Qq}^4}^{[1]} \approx 0.1$, which is the largest one-loop coefficient for $\rho_{V_{Qq}^4}$ in the mass range $m_Q a \leq 3$. This procedure yields a systematic error of 0.7%, which we take for both charm and bottom decay constants.

The decay-constant ratios f_{B_s}/f_{B^+} and f_{D_s}/f_{D^+} depend on the corresponding ratios of $\rho_{A_{Qs}^4}/\rho_{A_{Qq}^4}$. These ratios differ from unity only because of the small variation of the $\rho_{A_{Qq}^4}$ with light valence mass, which is described in Sec. V. We take the variation of the $\rho_{A_{Qq}^4}$ with light valence mass at $a \approx 0.09$ fm as the error. This yields an error of 0.1% for both bottom and charm.

The dominant corrections in the heavy-light renormalization factor as defined in Eq. (2.5) are due to $Z_{V_{qq}^4}$ and $Z_{V_{QQ}^4}$ which are calculated nonperturbatively. The values (and errors) for $Z_{V_{qq}^4}$ and $Z_{V_{QQ}^4}$ are listed in Tables IX and XI, respectively. To obtain the error in $Z_{V_{Qq}^4} = \sqrt{Z_{V_{qq}^4} Z_{V_{QQ}^4}}$ we add the statistical errors in $Z_{V_{qq}^4}$ and $Z_{V_{QQ}^4}$ in quadrature. The error on $Z_{V_{Qq}^4}$ is dominated by the error on $Z_{V_{qq}^4}$. The errors are largest, 1.3%, on the $a \approx 0.09$ fm ensemble, and they are about the same for both charm and bottom on the two finest ensembles used to obtain our main decay-constant results. Hence we use 1.3% as our estimate for the uncertainty in $Z_{V_{Qq}^4}$.

I. Finite-volume effects

To study finite-volume effects, we use the chiral fit function with heavy-light hyperfine and flavor splittings included [Eq. (6.20)], since the effects are known to be larger with the splittings than without [82]. The central fit includes the (one-loop) finite-volume corrections, Eq. (6.21), on the lattice data, and then takes the infinite volume limit when extracting the final results for the decay constants. We then take the larger of the following two values as our estimate of the finite-volume error:

V1. The difference between the central result and the result from a chiral fit in which the finite-volume corrections are omitted.

V2. The largest finite-volume correction to the relevant data points, as determined by the central fit. For ϕ_{D^+} and ϕ_{B^+} , the “relevant data points” are the ones on each ensemble with the lightest valence mass, i.e., those closest to the chirally extrapolated point. For ϕ_{D_s} and ϕ_{B_s} , the relevant points are the ones on each ensemble with valence mass closest to m_s .

Method V1 gives a larger difference for ϕ_{D_s} and ϕ_{B_s} ; method V2 gives a larger difference for ϕ_{D^+} and ϕ_{B^+} and the ratios. The resulting values are shown in Table XIII. Note that our choices are conservative because we correct for the (one-loop) finite-volume errors, but nevertheless take the full size of these effects as our error.

VIII. RESULTS AND CONCLUSIONS

After adding the error estimates described in the previous section in quadrature, we obtain

$$f_{B^+} = 196.9(9.1) \text{ MeV}, \quad (8.1)$$

$$f_{B_s} = 242.0(10.0) \text{ MeV}, \quad (8.2)$$

$$f_{B_s}/f_{B^+} = 1.229(0.026), \quad (8.3)$$

$$f_{D^+} = 218.9(11.3) \text{ MeV}, \quad (8.4)$$

$$f_{D_s} = 260.1(10.8) \text{ MeV}, \quad (8.5)$$

$$f_{D_s}/f_{D^+} = 1.188(0.025). \quad (8.6)$$

Since our most reliable method of determining discretization errors combines them with statistical errors, we do not quote separate statistical and systematic errors.

Figure 12 shows a comparison of our results for charmed decay constants with other lattice QCD calculations and with experiment. Our results agree with the only other

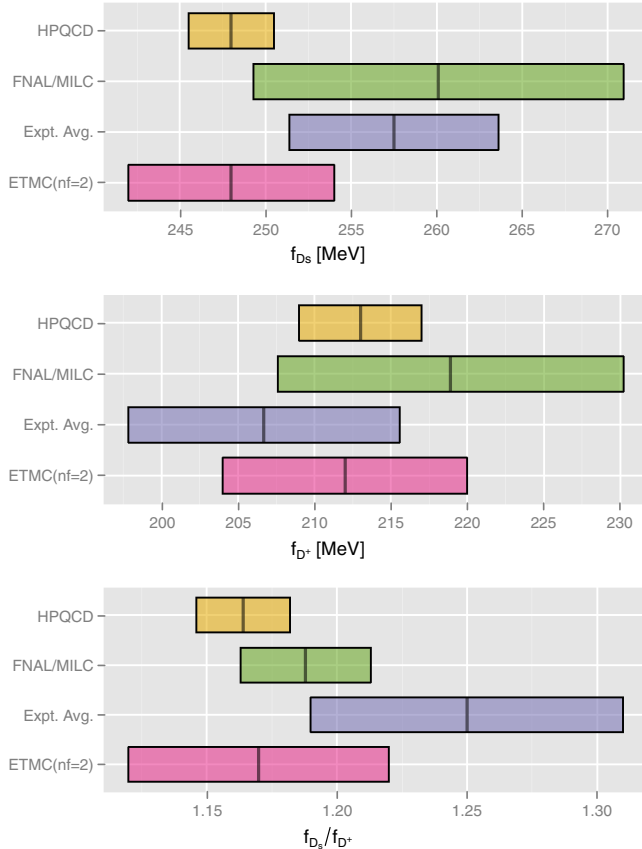


FIG. 12 (color online). Comparison of f_D and f_{D_s} with other two- and three-flavor lattice QCD calculations and with experiment. Results shown come from Refs. [53,99–106]. The HPQCD f_D value is computed from their update to f_{D_s} and their earlier result for the ratio f_{D_s}/f_D .

three-flavor lattice QCD determination from the HPQCD Collaboration [99], which is obtained with HISQ staggered valence quarks and Asqtad staggered sea quarks. (The difference in f_{D_s} is a bit greater than 1σ .) They are also consistent with the two-flavor results of the ETM Collaboration using twisted-mass Wilson fermions [100], although the ETM error budget does not include an estimate of the uncertainty due to quenching the strange quark. One can also compare with “experimental” determinations of f_D and f_{D_s} if one assumes CKM unitarity to obtain the matrix elements $|V_{cd}|$ and $|V_{cs}|$. For the D meson, Rosner and Stone combine CLEO’s measurement of the branching fraction $\mathcal{B}(D^+ \rightarrow \mu^+ \nu)$ [101] with the latest determination of $|V_{cd}|$ from the PDG [54] to obtain $f_D = 206.7(8.9) \text{ MeV}$ [53]. For the D_s meson, they average CLEO and Belle results for $\mathcal{B}(D_s^+ \rightarrow \mu^+ \nu)$ [102,103] with CLEO and BABAR results for $\mathcal{B}(D_s^+ \rightarrow \tau^+ \nu)$ [102,104–106] to obtain a combined average for the two decay channels of $f_{D_s} = 257.5(6.1) \text{ MeV}$ [53]. The Heavy Flavor Averaging Group obtains a similar average, $f_{D_s} = 257.3(5.3) \text{ MeV}$ [107]. Our results are consistent with these values, confirming standard model expectations at the $\sim 5\%$ level.

Figure 13 shows a similar comparison of our results for bottom meson decay constants with other lattice QCD calculations. Our results agree with the published three-flavor determination using NRQCD b quarks and Asqtad staggered light quarks of the HPQCD Collaboration [108], but are only marginally consistent with HPQCD’s more recent calculation of f_{B_s} using HISQ light valence quarks [109]. Our results are also consistent with the two-flavor results of the ETM Collaboration [100], who use Wilson heavy quarks and interpolate between the charm-mass region and the static limit to obtain results for bottom. Further, our result for the ratio f_{B_s}/f_B also agrees with the significantly less precise three-flavor determination using static b quarks and domain-wall light quarks by the RBC and UKQCD Collaborations [110].

For the D system the largest uncertainties in our current calculation stem from heavy-quark discretization, while the chiral extrapolation, the Z_V factors, excited states, heavy-quark tuning, and the chiral-continuum extrapolation play important but subdominant roles. For the B system, heavy-quark tuning, statistics, and excited states are the sources of the largest errors, while the Z_V factors and the chiral-continuum extrapolation (incorporating our estimate of heavy-quark discretization effects) are next in size. Recall that a novel feature of our work is the treatment of heavy-quark discretization effects, via the functions f_i in Eq. (2.4), and priors constraining the chiral-continuum fits to follow this form. At tree level, we have explicit calculations of the mismatch, some of which appeared already in Ref. [36] and all of which are compiled in Ref. [63]. Beyond the tree level, the continuum and static limits can be used to constrain the functional form. That

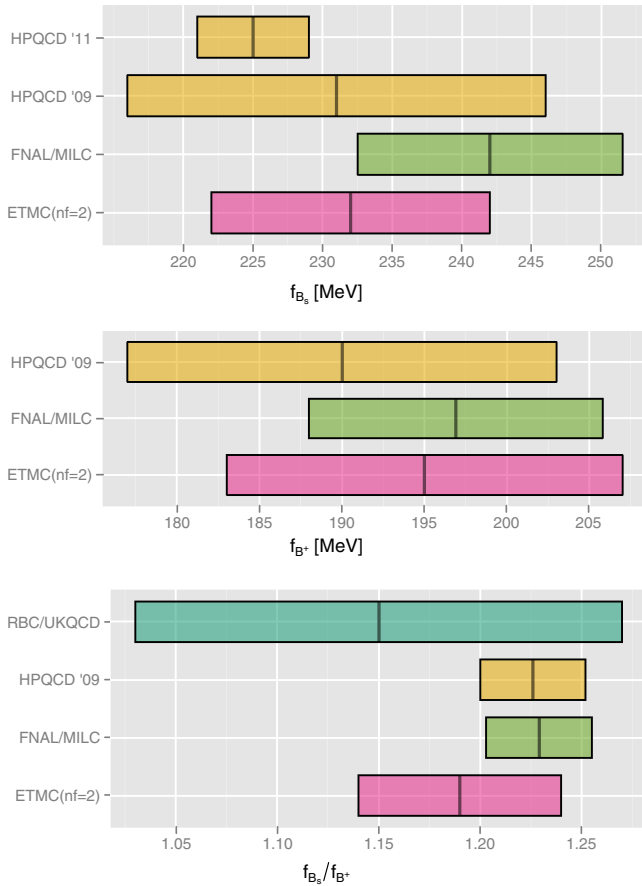


FIG. 13 (color online). Comparison of f_B and f_{B_s} with other two- and three-flavor lattice QCD calculations. Results shown come from Refs. [100,108–110]. In the case of f_{B_s} , HPQCD has two separate calculations using NRQCD b quarks and using HISQ b quarks; we show both the published NRQCD result (HPQCD '09) and the more recent HISQ result (HPQCD '11) in the plot above.

said, the theoretical guidance of the priors cannot be highly effective in an analysis, such as this, with only two lattice spacings. Indeed, the quoted heavy-quark discretization errors are similar to less sophisticated power-counting estimates.

While completing this analysis, we began runs to generate data that will address the main sources of uncertainty reported here. The new data set will contain 4 times the configurations used here to reduce the statistical errors in the correlation functions and, thus, directly improve the decay amplitudes, the determinations of the hopping parameters κ_c and κ_b , and the renormalization factors $Z_{V_{qq}^4}$ and $Z_{V_{qq}^4}$, all of which feed into the decay constant. Our new data will also encompass two finer lattice spacings of $a \approx 0.06$ fm and $a \approx 0.045$ fm, in order to explicitly reduce light- and heavy-quark discretization errors and better control the continuum extrapolation. With four lattice spacings, our new method of heavy-quark discretization priors will be put to a more stringent test. The new runs will

also include light valence- and sea-quark masses down to $\sim m_s/20$ in order to better control the chiral extrapolation to the physical d and u quark masses.

In order to reduce errors further, we will have to eliminate the errors from the matching factors and from quenching the charmed quark. The MILC Collaboration [111] is generating ensembles with $2 + 1 + 1$ flavors of sea quarks with the HISQ action, with plans to provide a range of lattice spacings and sea-quark masses equal to or more extensive than the $2 + 1$ Asqtad ensembles. Use of the HISQ action for the charm valence quark will allow us to further reduce many of the uncertainties, and it will provide the particularly nice advantage that one can use the local pseudoscalar density without multiplicative renormalization to obtain the continuum matrix element [112]. In several years, once the full suite of HISQ ensembles with several sea-quark masses and lattice spacings has been analyzed, we expect to obtain percent-level errors for both B - and D -meson decay constants. This will enable precise tests of the standard model and may help to reveal the presence of new physics in the quark-flavor sector.

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APPENDIX A: HEAVY-QUARK DISCRETIZATION EFFECTS

We are using the heavy-quark Lagrangian as given in [36], with $\kappa_t = \kappa_s$ (or, equivalently, $\zeta = 1$), $r_s = 1$, and $c_B = c_E = c_{\text{SW}}$. This amounts to the Sheikholeslami-Wohlert Lagrangian [35] for Wilson fermions [62]. The current has a heavy quark of this type, rotated as in Eq. (4.2) [cf. Eqs. (7.8)–(7.10) of Ref. [36]], and a staggered light quark. At the tree level, the heavy-quark rotation is the same no matter what the other quark is. The discretization effects are estimated from a (continuum) effective field theory [39–41], as shown explicitly for decay constants in Eqs. (8.7)–(8.12) of Ref. [39].

1. Theory

Both QCD and lattice gauge theory can be described via

$$\mathcal{L}_{\text{QCD}} \doteq \mathcal{L}_{\text{HQET}} = \sum_i \mathcal{C}_i^{\text{cont}}(m_Q) \mathcal{O}_i, \quad (\text{A1})$$

$$\mathcal{L}_{\text{LGT}} \doteq \mathcal{L}_{\text{HQET}(m_0a)} = \sum_i \mathcal{C}_i^{\text{lat}}(m_Q, m_0a) \mathcal{O}_i, \quad (\text{A2})$$

where the $\mathcal{C}_i$ are short-distance coefficients and the $\mathcal{O}_i$ are operators describing the long-distance physics. The coefficients have dimension $4 - \dim \mathcal{O}_i$. For lattice gauge theory, they depend on m_0a , which is a ratio of short distances a and $1/m_Q$. The effective-theory operators $\mathcal{O}_i$ in Eqs. (A1) and (A2) are the same.

The error from each term is simply the difference

$$\text{error}_i = |[\mathcal{C}_i^{\text{lat}}(m_Q, m_0a) - \mathcal{C}_i^{\text{cont}}(m_Q)] \mathcal{O}_i|. \quad (\text{A3})$$

The relative error in our matrix elements can be estimated by setting $\langle \mathcal{O}_i \rangle \sim \Lambda_{\text{QCD}}^{\dim \mathcal{O}_i - 4}$; choices for the QCD scale Λ_{QCD} are discussed below. The coefficient mismatch can be written

$$\mathcal{C}_i^{\text{lat}}(m_Q, m_0a) - \mathcal{C}_i^{\text{cont}}(m_Q) = a^{\dim \mathcal{O}_i - 4} f_i(m_0a). \quad (\text{A4})$$

This recovers the usual counting of powers of a (familiar from Symanzik [37,38]), but maintaining the full m_0a dependence. The final expression for the discretization errors is then

$$\text{error}_i \propto f_i(m_0a) (a \Lambda_{\text{QCD}})^{\dim \mathcal{O}_i - 4}. \quad (\text{A5})$$

For Wilson fermions, $\lim_{m_0a \rightarrow 0} f_i = \text{constant}$ (whereas in lattice NRQCD without fine-tuning, this is not the case). We have explicit calculations of the f_i for the $O(a)$ and $O(a^2)$ errors at the tree level [36,63]. The next subsection discusses how to use them to guide a continuum-limit extrapolation of the $O(\alpha_s a)$ and $O(a^2)$ errors.

Equations (A1) and (A2) can be generalized to currents. For the axial-vector current,

$$\begin{aligned} \mathcal{A}^\mu &\doteq C_{A\perp}^{\text{cont}}(m_Q) \bar{q} i \gamma_\perp^\mu \gamma_5 h_\nu - C_{A\parallel}^{\text{cont}}(m_Q) v^\mu \bar{q} \gamma_5 h_\nu \\ &\quad - \sum_i B_{Ai}^{\text{cont}}(m_Q) \mathcal{Q}_{Ai}^\mu, \end{aligned} \quad (\text{A6})$$

$$\begin{aligned} A_{\text{lat}}^\mu &\doteq C_{A\perp}^{\text{lat}}(m_Q, m_0a) \bar{q} i \gamma_\perp^\mu \gamma_5 h_\nu - C_{A\parallel}^{\text{lat}}(m_Q, m_0a) v^\mu \bar{q} \gamma_5 h_\nu \\ &\quad - \sum_i B_{Ai}^{\text{lat}}(m_Q, m_0a) \mathcal{Q}_{Ai}^\mu, \end{aligned} \quad (\text{A7})$$

and $\doteq$ again means in the sense of matrix elements. Here v^μ selects the temporal component and $\perp$ the spatial, and the list of dimension-4 operators $\mathcal{Q}$ can be found in Refs. [40].

The matrix element of the temporal component of the axial-vector current [cf. Eq. (4.7)] is normalized by multiplying with $Z_{A^4} = C_{A\parallel}^{\text{cont}}/C_{A\parallel}^{\text{lat}}$. The current mismatch then leads to errors

$$a^{\dim \mathcal{Q}_i - 3} f_i(m_0a) = Z_{A^4} B_{Ai}^{\text{lat}} - B_{Ai}^{\text{cont}}, \quad (\text{A8})$$

with the sum running over the two operators $\mathcal{Q}$ that point in the temporal direction [40].

2. Error estimation

The total error from heavy-quark discretization effects is then

$$\text{error} = \sum_i z_i (a \Lambda_{\text{QCD}})^{s_i} f_i(m_0a), \quad (\text{A9})$$

where the sum runs over Lagrangian operators $\mathcal{O}_i$ of dimension 5 and 6 and current operators $\mathcal{Q}_i$ of dimension 4 and 5, $s_i = \dim \mathcal{O}_i - 4$ or $\dim \mathcal{Q}_i - 3$, and the z_i are unknown coefficients. The functions f_i (summarized below) have been computed for $O(a^2)$ and estimated for $O(\alpha_s a)$. We omit contributions of order $\alpha_s^l a^2$, whether from extra operators or from iterating to second order operators with coefficients of order $\alpha_s a$.

In the past, we have taken a very conservative $\Lambda_{\text{QCD}} = 700$ MeV and assumed a Gaussian distribution for the z_i centered on 0 and of width 1. This amounts to treating the discretization errors as independent and adding them in quadrature. It also implicitly assumes that the data have nothing to say about the size or relative importance of the terms.

Here, however, we incorporate these errors into the chiral-continuum extrapolation, discussed in Sec. VI. This means that the z_i are now constrained fit parameters, with prior constraints discussed in Sec. VI.

The f_i are collected next.

a. $O(a^2)$ errors

We start with these, because explicit expressions for the functions $f_i(m_0a)$ are available. The Lagrangian leads to

two bilinears, $\bar{h}\mathbf{D} \cdot \mathbf{E}h$ and $\bar{h}i\mathbf{\Sigma} \cdot [\mathbf{D} \times \mathbf{E}]h$, and many four-quark operators. At the tree level the coefficients of all four-quark operators vanish, the coefficients of the two bilinears are the same, and the mismatch function is

$$f_E(m_0a) = \frac{1}{8m_E^2a^2} - \frac{1}{2(2m_2a)^2}. \quad (\text{A10})$$

Using explicit expressions for $1/m_2$ [36] and $1/m_E^2$ [63], one finds

$$f_E(m_0a) = \frac{1}{2} \left[\frac{c_E(1+m_0a) - 1}{m_0a(2+m_0a)(1+m_0a)} - \frac{1}{4(1+m_0a)^2} \right]. \quad (\text{A11})$$

We are using $c_E = 1$, so

$$f_E(m_0a) = \frac{2 + 3m_0a}{8(2 + m_0a)(1 + m_0a)^2}. \quad (\text{A12})$$

With no further assumptions, this term enters twice independently, so we take the width of this prior to be $\sqrt{2}$ rather than 1.

The current leads to three more terms with nonzero coefficients, $\bar{q}\Gamma\mathbf{D}^2h$, $\bar{q}\Gamma i\mathbf{\Sigma} \cdot \mathbf{B}h$, and $\bar{q}\Gamma\boldsymbol{\alpha} \cdot \mathbf{E}h$, which can be deduced from Eq. (A17) of Ref. [36]. Their coefficients can be read off from Eq. (A19). When $c_B = r_s$ the first two share the same coefficient,

$$\begin{aligned} f_X(m_0a) &= \frac{1}{8m_X^2a^2} - \frac{\zeta d_1(1+m_0a)}{m_0a(2+m_0a)} - \frac{1}{2(2m_2a)^2} \\ &= \frac{1}{2} \left[\frac{1}{(2+m_0a)(1+m_0a)} + \frac{1}{2(1+m_0a)} \right. \\ &\quad \left. - \frac{1}{4(1+m_0a)^2} - \frac{1}{(2+m_0a)^2} \right] \\ &= \frac{1}{2} \left[\frac{1}{2(1+m_0a)} - \left(\frac{m_0a}{2(2+m_0a)(1+m_0a)} \right)^2 \right], \end{aligned} \quad (\text{A13})$$

where the last term in the second expression comes from using the tree-level d_1 (as we do in the simulations). Because of the twofold appearance, we again take the prior width to be $\sqrt{2}$.

For $\bar{q}\Gamma\boldsymbol{\alpha} \cdot \mathbf{E}h$

$$\begin{aligned} f_Y(m_0a) &= \frac{1}{2} \left[\frac{d_1}{m_2a} - \frac{\zeta(1-c_E)(1+m_0a)}{m_0a(2+m_0a)} \right] \\ &= \frac{2 + 4m_0a + (m_0a)^2}{4(1+m_0a)^2(2+m_0a)^2}, \end{aligned} \quad (\text{A14})$$

where the last line reflects the choices made for c_E and d_1 .

TABLE XIV. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from analysis I fits of the charm correlators at lattice spacing $a \approx 0.09$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0031/0.031	0.0031	0.7523(0.0016)	0.0857(0.0015)	58/48	0.23
0.0031/0.031	0.0044	0.7553(0.0014)	0.0873(0.0013)	56/48	0.28
0.0031/0.031	0.0062	0.7589(0.0011)	0.0890(0.0011)	55/48	0.33
0.0031/0.031	0.0087	0.7634(0.0009)	0.0910(0.0009)	53/48	0.38
0.0031/0.031	0.0124	0.7699(0.0007)	0.0936(0.0007)	53/48	0.41
0.0031/0.031	0.0186	0.7807(0.0005)	0.0978(0.0006)	52/48	0.44
0.0031/0.031	0.0272	0.7954(0.0004)	0.1030(0.0005)	50/48	0.5
0.0031/0.031	0.031	0.8018(0.0004)	0.1052(0.0004)	50/48	0.5
0.0062/0.031	0.0031	0.7541(0.0030)	0.0875(0.0027)	56/48	0.37
0.0062/0.031	0.0044	0.7577(0.0023)	0.0899(0.0021)	52/48	0.49
0.0062/0.031	0.0062	0.7613(0.0019)	0.0917(0.0018)	50/48	0.58
0.0062/0.031	0.0087	0.7654(0.0015)	0.0933(0.0015)	58/51	0.43
0.0062/0.031	0.0124	0.7712(0.0012)	0.0952(0.0012)	52/48	0.48
0.0062/0.031	0.0186	0.7810(0.0009)	0.0985(0.0010)	56/48	0.37
0.0062/0.031	0.0272	0.7952(0.0006)	0.1032(0.0008)	59/48	0.28
0.0062/0.031	0.031	0.8015(0.0005)	0.1052(0.0007)	60/48	0.25
0.0124/0.031	0.0031	0.7551(0.0038)	0.0930(0.0036)	60/48	0.27
0.0124/0.031	0.0042	0.7554(0.0031)	0.0926(0.0028)	65/48	0.15
0.0124/0.031	0.0062	0.7574(0.0023)	0.0929(0.0021)	65/48	0.16
0.0124/0.031	0.0087	0.7608(0.0017)	0.0938(0.0015)	59/48	0.28
0.0124/0.031	0.0124	0.7666(0.0013)	0.0957(0.0012)	49/48	0.63
0.0124/0.031	0.0186	0.7766(0.0008)	0.0991(0.0009)	42/48	0.85
0.0124/0.031	0.0272	0.7907(0.0006)	0.1038(0.0007)	48/48	0.64
0.0124/0.031	0.031	0.7969(0.0005)	0.1058(0.0006)	53/48	0.47

b. $O(\alpha_s a)$ and $O(a^3)$ errors

Here the mismatch functions $f_i(m_0 a)$ start at order α_s , and we do not have explicit expressions for them. We take unimproved tree-level coefficients as a guide to the combinatoric factors and the asymptotic behavior as $m_0 a \rightarrow 0$ and $m_0 a \rightarrow \infty$.

The Lagrangian leads to two bilinears, the kinetic energy $\mathcal{O}_2 = \bar{h} \mathbf{D}^2 h$ and the chromomagnetic moment $\mathcal{O}_B = \bar{h} i \mathbf{\Sigma} \cdot \mathbf{B} h$. We match the former nonperturbatively, by identifying the meson's kinetic mass with the physical mass; the discretization error f_2 stems, therefore, from discretization effects in M_2 .

The computed kinetic meson mass is

$$M_2 = m_2(\kappa) + \text{continuum binding energy} + \delta M_2, \quad (\text{A15})$$

where [58]

$$\delta M_2 = \frac{\bar{\Lambda}^2}{6m_Q} \left[5 \left(\frac{m_2^3}{m_4^3} - 1 \right) + 4w_4(m_2 a)^3 \right], \quad (\text{A16})$$

and m_2 , m_4 , and w_4 are functions of $m_0 a$ and, hence, κ . (See Refs. [36,63] for explicit expressions.) Equating M_2 to a physical meson mass means that we choose κ such that $m_2(\kappa) + \delta M_2 = m_Q$, thereby making in ϕ a relative error

$$\begin{aligned} \text{error}_2 &= \bar{\Lambda} \left(\frac{1}{2m_2} - \frac{1}{2m_Q} \right) \\ &= \bar{\Lambda} \left(\frac{1}{2m_Q - 2\delta M_2} - \frac{1}{2m_Q} \right) \approx \bar{\Lambda} \frac{\delta M_2}{2m_Q^2}. \end{aligned} \quad (\text{A17})$$

TABLE XV. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from analysis I fits of the charm correlators at lattice spacing $a \approx 0.12$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.005/0.050	0.005	0.9943(0.0032)	0.1436(0.0030)	30/30	0.52
0.005/0.050	0.007	0.9977(0.0024)	0.1453(0.0024)	29/30	0.6
0.005/0.050	0.01	1.0026(0.0018)	0.1477(0.0019)	28/30	0.64
0.005/0.050	0.014	1.0090(0.0016)	0.1508(0.0017)	28/30	0.64
0.005/0.050	0.02	1.0186(0.0013)	0.1551(0.0015)	29/30	0.58
0.005/0.050	0.03	1.0345(0.0010)	0.1620(0.0012)	33/30	0.42
0.005/0.050	0.0415	1.0526(0.0008)	0.1694(0.0010)	36/30	0.27
0.007/0.050	0.005	0.9948(0.0035)	0.1442(0.0035)	17/30	0.98
0.007/0.050	0.007	0.9975(0.0027)	0.1455(0.0028)	19/30	0.95
0.007/0.050	0.01	1.0019(0.0021)	0.1476(0.0021)	22/30	0.89
0.007/0.050	0.014	1.0081(0.0016)	0.1504(0.0017)	24/30	0.83
0.007/0.050	0.02	1.0178(0.0012)	0.1547(0.0014)	23/30	0.85
0.007/0.050	0.03	1.0338(0.0009)	0.1615(0.0010)	20/30	0.94
0.007/0.050	0.0415	1.0520(0.0007)	0.1687(0.0008)	19/30	0.95
0.010/0.050	0.005	0.9958(0.0039)	0.1461(0.0041)	15/30	0.99
0.010/0.050	0.007	1.0000(0.0031)	0.1486(0.0032)	20/30	0.94
0.010/0.050	0.01	1.0057(0.0024)	0.1516(0.0026)	26/30	0.75
0.010/0.050	0.014	1.0126(0.0019)	0.1549(0.0021)	29/27	0.41
0.010/0.050	0.02	1.0226(0.0015)	0.1594(0.0017)	33/30	0.39
0.010/0.050	0.03	1.0387(0.0011)	0.1662(0.0014)	31/30	0.5
0.010/0.050	0.0415	1.0567(0.0008)	0.1733(0.0011)	27/30	0.68
0.020/0.050	0.005	0.9942(0.0046)	0.1537(0.0050)	49/30	0.036
0.020/0.050	0.007	0.9959(0.0036)	0.1533(0.0039)	49/30	0.036
0.020/0.050	0.01	0.9987(0.0027)	0.1532(0.0031)	48/30	0.051
0.020/0.050	0.014	1.0037(0.0021)	0.1543(0.0024)	45/30	0.075
0.020/0.050	0.02	1.0124(0.0016)	0.1575(0.0019)	43/30	0.11
0.020/0.050	0.03	1.0274(0.0011)	0.1632(0.0014)	37/30	0.27
0.020/0.050	0.0415	1.0447(0.0009)	0.1695(0.0012)	32/30	0.48
0.030/0.050	0.005	0.9830(0.0042)	0.1475(0.0042)	33/30	0.39
0.030/0.050	0.007	0.9853(0.0033)	0.1485(0.0033)	33/30	0.4
0.030/0.050	0.01	0.9897(0.0025)	0.1505(0.0025)	32/30	0.47
0.030/0.050	0.014	0.9960(0.0020)	0.1534(0.0020)	31/30	0.53
0.030/0.050	0.02	1.0054(0.0015)	0.1574(0.0016)	32/30	0.46
0.030/0.050	0.03	1.0205(0.0011)	0.1633(0.0012)	37/30	0.27
0.030/0.050	0.0415	1.0376(0.0009)	0.1695(0.0010)	40/30	0.15

TABLE XVI. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from analysis I fits of the charm correlators at lattice spacing $a \approx 0.15$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0097/0.0484	0.0048	1.1659(0.0044)	0.1979(0.0052)	20/20	0.5
0.0097/0.0484	0.007	1.1710(0.0034)	0.2017(0.0040)	22/20	0.37
0.0097/0.0484	0.0097	1.1768(0.0027)	0.2054(0.0032)	25/20	0.26
0.0097/0.0484	0.0194	1.1951(0.0016)	0.2159(0.0020)	25/20	0.26
0.0097/0.0484	0.029	1.2117(0.0012)	0.2242(0.0015)	20/20	0.51
0.0097/0.0484	0.0484	1.2432(0.0009)	0.2385(0.0012)	15/20	0.79
0.0194/0.0484	0.0048	1.1726(0.0046)	0.2106(0.0052)	23/20	0.35
0.0194/0.0484	0.007	1.1749(0.0036)	0.2105(0.0041)	23/20	0.35
0.0194/0.0484	0.0097	1.1785(0.0028)	0.2113(0.0031)	23/20	0.32
0.0194/0.0484	0.0194	1.1935(0.0016)	0.2174(0.0020)	30/20	0.092
0.0194/0.0484	0.029	1.2091(0.0013)	0.2244(0.0016)	32/20	0.055
0.0194/0.0484	0.0484	1.2400(0.0010)	0.2381(0.0013)	27/20	0.17
0.0290/0.0484	0.0048	1.1613(0.0044)	0.1975(0.0049)	17/20	0.72
0.0290/0.0484	0.007	1.1660(0.0034)	0.2010(0.0040)	18/20	0.64
0.0290/0.0484	0.0097	1.1717(0.0026)	0.2049(0.0031)	21/20	0.47
0.0290/0.0484	0.0194	1.1896(0.0015)	0.2151(0.0019)	24/20	0.3
0.0290/0.0484	0.029	1.2058(0.0011)	0.2229(0.0015)	23/20	0.32
0.0290/0.0484	0.0484	1.2368(0.0008)	0.2364(0.0011)	20/20	0.49

TABLE XVII. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from analysis I fits of the bottom correlators at lattice spacing $a \approx 0.09$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0031/0.031	0.0031	1.6509(0.0018)	0.1359(0.0016)	41/39	0.48
0.0031/0.031	0.0044	1.6532(0.0016)	0.1378(0.0015)	40/39	0.51
0.0031/0.031	0.0062	1.6562(0.0015)	0.1402(0.0014)	40/39	0.49
0.0031/0.031	0.0087	1.6601(0.0013)	0.1433(0.0014)	42/39	0.42
0.0031/0.031	0.0124	1.6659(0.0012)	0.1475(0.0013)	45/39	0.31
0.0031/0.031	0.0186	1.6752(0.0011)	0.1542(0.0012)	47/39	0.23
0.0031/0.031	0.0272	1.6879(0.0009)	0.1628(0.0011)	49/39	0.19
0.0031/0.031	0.031	1.6934(0.0009)	0.1664(0.0011)	49/39	0.18
0.0062/0.031	0.0031	1.6539(0.0046)	0.1358(0.0051)	40/39	0.56
0.0062/0.031	0.0044	1.6557(0.0039)	0.1377(0.0044)	37/39	0.68
0.0062/0.031	0.0062	1.6584(0.0032)	0.1402(0.0037)	34/39	0.77
0.0062/0.031	0.0087	1.6620(0.0027)	0.1434(0.0031)	34/39	0.8
0.0062/0.031	0.0124	1.6675(0.0022)	0.1480(0.0026)	36/39	0.72
0.0062/0.031	0.0186	1.6767(0.0018)	0.1550(0.0022)	41/39	0.53
0.0062/0.031	0.0272	1.6892(0.0014)	0.1637(0.0019)	45/39	0.37
0.0062/0.031	0.031	1.6946(0.0014)	0.1672(0.0018)	45/39	0.35
0.0124/0.031	0.0031	1.6532(0.0036)	0.1387(0.0038)	52/39	0.16
0.0124/0.031	0.0042	1.6550(0.0033)	0.1407(0.0034)	48/39	0.27
0.0124/0.031	0.0062	1.6576(0.0030)	0.1432(0.0031)	40/39	0.55
0.0124/0.031	0.0087	1.6606(0.0027)	0.1456(0.0029)	35/39	0.77
0.0124/0.031	0.0124	1.6650(0.0024)	0.1488(0.0027)	33/39	0.84
0.0124/0.031	0.0186	1.6730(0.0019)	0.1544(0.0023)	36/39	0.73
0.0124/0.031	0.0272	1.6847(0.0016)	0.1623(0.0021)	42/39	0.48
0.0124/0.031	0.031	1.6900(0.0015)	0.1657(0.0020)	45/39	0.38

The right-most expression is $(a\bar{\Lambda})^3 f_2(m_0 a)$, $f_2 = \square/12(m_2 a)^3$, where $\square$ is the bracket in Eq. (A16). It is formally smaller than the other errors considered here— f_2 is of order 1 for all $m_0 a$. Numerically, however, it is not much smaller.

At the tree level the chromomagnetic mismatch is

$$f_B^{[0]}(m_0 a) = \frac{c_B - 1}{2(1 + m_0 a)}. \quad (\text{A18})$$

This has the right asymptotic behavior in both limits, so our Ansatz for the one-loop mismatch function is simply

$$f_B(m_0 a) = \frac{\alpha_s}{2(1 + m_0 a)}, \quad (\text{A19})$$

and error_B is this function multiplied by $a\Lambda$. We take $\alpha_s = 0.288$ on the $a \approx 0.12$ fm ensembles, which is the value determined for α_V from the plaquette [79] with one-loop running to scale $q^* = 2.5/a$. On other ensembles, α_s is found by assuming that the measured average taste splitting goes like $\alpha_s^2 a^2$ (with a determined from r_1/a). This gives α_s values that track $\alpha_V(q^* = 2.5/a)$ quite well, which is why we make that q^* choice. The results are rather insensitive to the details here. For example, using $\alpha_s = 0.325$ on the $a \approx 0.12$ fm ensembles, which corresponds to $q^* = 2.0/a$, increases the error estimate by less than 0.6 MeV for f_{D^+} and less than 0.25 MeV for f_{B^+} .

The current leads to one more term, with tree-level mismatch function

TABLE XVIII. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from analysis I fits of the bottom correlators at lattice spacing $a \approx 0.12$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.005/0.050	0.005	1.9170(0.0044)	0.2236(0.0050)	45/27	0.03
0.005/0.050	0.007	1.9197(0.0039)	0.2263(0.0046)	46/27	0.022
0.005/0.050	0.01	1.9235(0.0033)	0.2300(0.0040)	46/27	0.021
0.005/0.050	0.014	1.9287(0.0029)	0.2347(0.0036)	45/27	0.027
0.005/0.050	0.02	1.9367(0.0024)	0.2418(0.0031)	43/27	0.046
0.005/0.050	0.03	1.9503(0.0020)	0.2532(0.0026)	39/27	0.096
0.005/0.050	0.0415	1.9657(0.0017)	0.2654(0.0023)	36/27	0.17
0.007/0.050	0.005	1.9147(0.0036)	0.2224(0.0039)	37/27	0.12
0.007/0.050	0.007	1.9177(0.0033)	0.2254(0.0037)	35/27	0.17
0.007/0.050	0.01	1.9219(0.0030)	0.2292(0.0036)	34/27	0.2
0.007/0.050	0.014	1.9272(0.0028)	0.2337(0.0037)	35/27	0.19
0.007/0.050	0.02	1.9351(0.0026)	0.2401(0.0037)	36/27	0.15
0.007/0.050	0.03	1.9485(0.0022)	0.2508(0.0035)	38/27	0.096
0.007/0.050	0.0415	1.9638(0.0019)	0.2628(0.0031)	40/27	0.07
0.010/0.050	0.005	1.9182(0.0047)	0.2254(0.0047)	30/27	0.4
0.010/0.050	0.007	1.9207(0.0041)	0.2284(0.0042)	32/27	0.29
0.010/0.050	0.01	1.9250(0.0035)	0.2328(0.0037)	36/27	0.18
0.010/0.050	0.014	1.9307(0.0030)	0.2383(0.0033)	39/27	0.097
0.010/0.050	0.02	1.9391(0.0025)	0.2457(0.0028)	43/27	0.048
0.010/0.050	0.03	1.9527(0.0020)	0.2569(0.0024)	47/27	0.02
0.010/0.050	0.0415	1.9682(0.0017)	0.2689(0.0021)	51/27	0.0092
0.020/0.050	0.005	1.9136(0.0060)	0.2278(0.0069)	33/27	0.27
0.020/0.050	0.007	1.9163(0.0050)	0.2305(0.0059)	33/27	0.28
0.020/0.050	0.01	1.9200(0.0042)	0.2340(0.0050)	31/27	0.36
0.020/0.050	0.014	1.9249(0.0036)	0.2381(0.0043)	29/27	0.47
0.020/0.050	0.02	1.9322(0.0031)	0.2437(0.0039)	28/27	0.52
0.020/0.050	0.03	1.9445(0.0027)	0.2526(0.0038)	30/27	0.42
0.020/0.050	0.0415	1.9590(0.0025)	0.2627(0.0039)	33/27	0.3
0.030/0.050	0.005	1.9030(0.0058)	0.2196(0.0073)	38/27	0.12
0.030/0.050	0.007	1.9058(0.0049)	0.2223(0.0064)	32/27	0.29
0.030/0.050	0.01	1.9099(0.0041)	0.2258(0.0056)	27/27	0.56
0.030/0.050	0.014	1.9155(0.0034)	0.2306(0.0048)	23/27	0.74
0.030/0.050	0.02	1.9239(0.0028)	0.2376(0.0040)	22/27	0.77
0.030/0.050	0.03	1.9372(0.0022)	0.2479(0.0034)	25/27	0.64
0.030/0.050	0.0415	1.9518(0.0019)	0.2585(0.0032)	28/27	0.49

$$f_3^{[0]}(m_0 a) = \frac{m_0 a}{2(2 + m_0 a)(1 + m_0 a)} - d_1, \quad (\text{A20})$$

and the tree-level d_1 is chosen so that $f_3^{[0]} = 0$. As with the mismatch function f_B , we would like to anticipate $f_3^{[1]}$ by setting $d_1^{[1]} = 0$ and multiplying the rest with α_s . But it is not generic that this vanishes as $m_0 a \rightarrow 0$. Therefore, we take

$$f_3(m_0 a) = \frac{\alpha_s}{2(2 + m_0 a)}, \quad (\text{A21})$$

which has the right asymptotic behavior. We take the prior width as $\sqrt{2}$, because A^4 has two such corrections [40].

3. Dispersion relation, Eq. (3.1)

We take a similar approach to the dispersion relation, Eq. (3.1), with the difference that we now know the sign of the leading effect.

The tree-level functions are

$$a_4^{[0]} = \frac{1}{(m_2^{[0]} a)^2} - \frac{m_1^{[0]} a}{(m_4^{[0]} a)^3}, \quad (\text{A22})$$

$$a_{4'}^{[0]} = m_1^{[0]} a w_4^{[0]}. \quad (\text{A23})$$

The binding energy enters A_4 and $A_{4'}$ via the meson's kinetic energy. Hence, the binding contributions are

$$A_4' = \frac{3m_1^{[0]} a}{m_2^{[0]} a (m_4^{[0]} a)^3} - \frac{2}{(m_2^{[0]} a)^3} - \frac{1}{(m_4^{[0]} a)^3}, \quad (\text{A24})$$

$$A_{4'}' = w_4^{[0]} \left(1 - \frac{m_1^{[0]} a}{m_2^{[0]} a} \right), \quad (\text{A25})$$

and in Eq. (3.4) the binding energy floats within a Gaussian prior described by $(\bar{\Lambda}, \sigma_{\bar{\Lambda}}) = (600, 400)$ MeV. This choice conservatively brackets the binding energy of a heavy-strange meson. For the higher-order perturbative contribution to the coefficients, we take the Ansätze based on the asymptotic behavior:

$$a_4^{[1]} = \frac{y_4 + z_4 \ln(1 + m_0 a)}{(1 + m_0 a)^2}, \quad (\text{A26})$$

$$a_{4'}^{[1]} = \frac{y_{4'} m_0 a + z_{4'} \ln(1 + m_0 a)}{1 + m_0 a}, \quad (\text{A27})$$

where the y 's and z 's float within Gaussian priors described by $(y_4, \sigma_{y_4}) = (3, 5)$, $(z_4, \sigma_{z_4}) = (1, 2)$, $(y_{4'}, \sigma_{y_{4'}}) = (0, 0)$, and $(z_{4'}, \sigma_{z_{4'}}) = (0, 2)$. The terms proportional to y_i stem from the $m_0 a \rightarrow 0$ limit, in which the renormalization of m_4 must coincide with that of m_1 , and $a_4 = m_1 a w_4$ must vanish like $m_0 a$. The terms proportional to z_i stem from the $m_0 a \rightarrow \infty$ limit, where the static limit is obtained. Except for $y_{4'}$, the numerical values have been chosen to be consistent with the one-loop experience for m_1 and m_2 [113]. We have set $y_{4'} \equiv 0$, because at small $m_0 a$ it is indistinguishable from the other term in $a_{4'}^{[1]}$, and our range of $m_0 a$ does not reach far into the region $m_0 a \gg 1$.

TABLE XIX. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from analysis I fits of the bottom correlators at lattice spacing $a \approx 0.15$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2} \phi_H$	χ^2/dof	p
0.0097/0.0484	0.0048	2.2553(0.0071)	0.3311(0.0115)	36/25	0.097
0.0097/0.0484	0.007	2.2576(0.0061)	0.3341(0.0102)	37/25	0.09
0.0097/0.0484	0.0097	2.2611(0.0052)	0.3389(0.0089)	36/25	0.1
0.0097/0.0484	0.0194	2.2757(0.0036)	0.3568(0.0063)	34/25	0.16
0.0097/0.0484	0.029	2.2901(0.0030)	0.3727(0.0053)	33/25	0.16
0.0097/0.0484	0.0484	2.3175(0.0023)	0.4002(0.0046)	35/25	0.12
0.0194/0.0484	0.0048	2.2296(0.0175)	0.2743(0.0416)	32/25	0.2
0.0194/0.0484	0.007	2.2349(0.0142)	0.2823(0.0357)	34/25	0.15
0.0194/0.0484	0.0097	2.2416(0.0118)	0.2917(0.0309)	36/25	0.1
0.0194/0.0484	0.0194	2.2639(0.0072)	0.3243(0.0202)	36/25	0.1
0.0194/0.0484	0.029	2.2819(0.0054)	0.3482(0.0152)	30/25	0.27
0.0194/0.0484	0.0484	2.3124(0.0038)	0.3839(0.0109)	24/25	0.59
0.0290/0.0484	0.0048	2.2402(0.0073)	0.3101(0.0123)	29/25	0.32
0.0290/0.0484	0.007	2.2464(0.0061)	0.3199(0.0104)	30/25	0.28
0.0290/0.0484	0.0097	2.2524(0.0052)	0.3289(0.0089)	31/25	0.25
0.0290/0.0484	0.0194	2.2695(0.0036)	0.3502(0.0066)	27/25	0.42
0.0290/0.0484	0.029	2.2847(0.0030)	0.3665(0.0058)	21/25	0.72
0.0290/0.0484	0.0484	2.3125(0.0025)	0.3939(0.0057)	18/25	0.87

APPENDIX B: TWO-POINT FIT RESULTS FROM ANALYSIS I

Here we present complete fit results using analysis I, as described in Sec. IV B, for the heavy-light pseudoscalar meson mass and renormalized decay constant. Results for all combinations of sea-quark mass, light valence-quark mass, and heavy-quark mass used in the chiral-continuum extrapolation are collected in Tables XIV, XV, XVI, XVII, XVIII, and XIX.

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- [1] M. Bona M. Ciuchini, E. Franco, V. Lubicz, G. Martinelli, F. Parodi, M. Pierini, C. Schiavi, L. Silvestrini, V. Sordini, A. Stocchi, C. Tarantino, and V. Vagnoni (UTfit Collaboration), *Phys. Lett. B* **687**, 61 (2010).
 - [2] A. Lenz, U. Nierste, J. Charles, S. Descotes-Genon, A. Jantsch, C. Kaufhold, H. Lacker, S. Monteil, V. Niess, and S. T'Jampens (CKMfitter Group), *Phys. Rev. D* **83**, 036004 (2011).
 - [3] E. Lunghi and A. Soni, *Phys. Lett. B* **697**, 323 (2011).
 - [4] J. Laiho, E. Lunghi, and R. Van de Water, Proc. Sci., FPCP2010 (2010) 040 [[arXiv:1102.3917](#)].
 - [5] K. Hara *et al.* (Belle Collaboration), *Phys. Rev. D* **82**, 071101 (2010).
 - [6] P. del Amo Sanchez *et al.* (BABAR Collaboration), in Proceedings of the 35th International Conference on High Energy Physics, ICHEP, Paris, 2010 [[arXiv:1008.0104](#)].
 - [7] M. Masuzawa, in Proceedings of IPAC, Kyoto, 2010, edited by K. Oide, <http://accelconf.web.cern.ch/accelconf/IPAC10/papers/frxbmh01.pdf>.
 - [8] T. Iijima, Search for Charged Higgs in $B \rightarrow \tau \nu$ and $D \rightarrow \tau \nu$ Decays, <http://kds.kek.jp/materialDisplay.py?contribId=5&sessionId=2&materialId=slides&confId=2865> (2009).
 - [9] B. O'Leary *et al.* (SuperB Collaboration), [arXiv:1008.1541](#).
 - [10] M.E. Biagini *et al.* (SuperB Collaboration), [arXiv:1009.6178](#).
 - [11] E. Lunghi and A. Soni, *Phys. Rev. Lett.* **104**, 251802 (2010).
 - [12] C.T.H. Davies *et al.* (HPQCD, UKQCD, MILC, and Fermilab Lattice Collaborations), *Phys. Rev. Lett.* **92**, 022001 (2004).
 - [13] L. Susskind, *Phys. Rev. D* **16**, 3031 (1977).
 - [14] H.S. Sharatchandra, H.J. Thun, and P. Weisz, *Nucl. Phys. B* **192**, 205 (1981).
 - [15] C. Aubin, C. Bernard, C. DeTar, J. Osborn, S. Gottlieb, E.B. Gregory, D. Toussaint, U.M. Heller, J.E. Hetrick, and R. Sugar (MILC Collaboration), *Phys. Rev. D* **70**, 114501 (2004).
 - [16] I.F. Allison C.T.H. Davies, A. Gray, A.S. Kronfeld, P.B. Mackenzie, and J.N. Simone (HPQCD, Fermilab Lattice, and UKQCD Collaborations), *Phys. Rev. Lett.* **94**, 172001 (2005).
 - [17] S. Prelovšek, *Phys. Rev. D* **73**, 014506 (2006).
 - [18] C. Bernard, *Phys. Rev. D* **73**, 114503 (2006).
 - [19] C. Bernard, C.E. DeTar, Z. Fu, and S. Prelovšek, *Phys. Rev. D* **76**, 094504 (2007).
 - [20] C. Aubin, J. Laiho, and R.S. Van de Water, *Phys. Rev. D* **77**, 114501 (2008).
 - [21] C. Bernard, M. Golterman, and Y. Shamir, *Phys. Rev. D* **73**, 114511 (2006).
 - [22] Y. Shamir, *Phys. Rev. D* **71**, 034509 (2005).
 - [23] Y. Shamir, *Phys. Rev. D* **75**, 054503 (2007).
 - [24] C. Bernard, M. Golterman, and Y. Shamir, *Phys. Rev. D* **77**, 074505 (2008).
 - [25] W.-J. Lee and S.R. Sharpe, *Phys. Rev. D* **60**, 114503 (1999).
 - [26] C. Aubin and C. Bernard, *Phys. Rev. D* **68**, 034014 (2003).
 - [27] S.R. Sharpe and R.S. Van de Water, *Phys. Rev. D* **71**, 114505 (2005).
 - [28] S.R. Sharpe, Proc. Sci., LAT2006 (2006) 022 [[arXiv:hep-lat/0610094](#)].
 - [29] A.S. Kronfeld, Proc. Sci., LAT2007 (2007) 016 [[arXiv:0711.0699](#)].
 - [30] M. Golterman, Proc. Sci., CONFINEMENT8 (2008) 014 [[arXiv:0812.3110](#)].
 - [31] A. Bazavov, D. Toussaint, C. Bernard, J. Laiho, C. DeTar, L. Levkova, M.B. Oktay, S. Gottlieb, U.M. Heller, J.E. Hetrick, P.B. Mackenzie, R. Sugar, and R.S. Van de Water, *Rev. Mod. Phys.* **82**, 1349 (2010).
 - [32] G.C. Donald, C.T.H. Davies, E. Follana, and A.S. Kronfeld, *Phys. Rev. D* **84**, 054504 (2011).
 - [33] J. Laiho, E. Lunghi, and R.S. Van de Water, *Phys. Rev. D* **81**, 034503 (2010).
 - [34] C.W. Bernard, T. Burch, K. Orginos, D. Toussaint, T.A. DeGrand, C. DeTar, S. Datta, S. Gottlieb, U.M. Heller, and R. Sugar, *Phys. Rev. D* **64**, 054506 (2001).
 - [35] B. Sheikholeslami and R. Wohlert, *Nucl. Phys. B* **259**, 572 (1985).
 - [36] A.X. El-Khadra, A.S. Kronfeld, and P.B. Mackenzie, *Phys. Rev. D* **55**, 3933 (1997).
 - [37] K. Symanzik, *Nucl. Phys. B* **226**, 187 (1983).
 - [38] K. Symanzik, *Nucl. Phys. B* **226**, 205 (1983).
 - [39] A.S. Kronfeld, *Phys. Rev. D* **62**, 014505 (2000).
 - [40] J. Harada, S. Hashimoto, K.-I. Ishikawa, A.S. Kronfeld, T. Onogi, and N. Yamada, *Phys. Rev. D* **65**, 094513 (2002); **71**, 019903(E) (2005).
 - [41] J. Harada, S. Hashimoto, A.S. Kronfeld, and T. Onogi, *Phys. Rev. D* **65**, 094514 (2002).
 - [42] C. Aubin and C. Bernard, *Phys. Rev. D* **73**, 014515 (2006).
 - [43] J. Laiho and R.S. Van de Water, *Phys. Rev. D* **73**, 054501 (2006).
 - [44] C. Aubin and C. Bernard, *Phys. Rev. D* **76**, 014002 (2007).
 - [45] A.X. El-Khadra, A.S. Kronfeld, P.B. Mackenzie, S.M. Ryan, and J.N. Simone, *Phys. Rev. D* **64**, 014502 (2001).
 - [46] A.X. El-Khadra, E. Gámiz, A.S. Kronfeld, and M.A. Nobes, Proc. Sci., LAT2007 (2007) 242 [[arXiv:0710.1437](#)].
 - [47] C. Aubin *et al.* (Fermilab Lattice, MILC, and HPQCD Collaborations), *Phys. Rev. Lett.* **95**, 122002 (2005).

- [48] C. Bernard *et al.* (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2006 (2006) 094.
- [49] C. Bernard, B. Billeter, C. DeTar, L. Levkova, S. Gottlieb, U. M. Heller, J. E. Hetrick, J. Osborn, D. B. Renner, D. Toussaint, and R. Sugar (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2007 (2007) 310.
- [50] C. Bernard, C. DeTar, M. Di Pierro, A. X. El-Khadra, R. T. Evans, E. D. Freeland, E. Gamiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, J. Simone, R. Sugar, D. Toussaint, and R. S. Van de Water (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LATTICE2008 (2008) 278 [[arXiv:0904.1895](#)].
- [51] A. Bazavov, C. Bernard, C. DeTar, E. D. Freeland, E. Gamiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. X. El-Khadra, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, M. B. Oktay, M. Di Pierro, J. N. Simone, R. Sugar, D. Toussaint, and R. S. Van de Water (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2009 (2009) 249 [[arXiv:0912.5221](#)].
- [52] J. Simone *et al.* (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LATTICE2010 (2010) 317.
- [53] J. L. Rosner and S. Stone, in Ref. [54], [arXiv:1002.1655](#).
- [54] K. Nakamura *et al.* (Particle Data Group), *J. Phys. G* **37**, 075021 (2010), and 2011 partial update for the 2012 edition.
- [55] C. Aubin, C. Bernard, C. DeTar, M. DiPierro, A. El-Khadra, S. Gottlieb, E. B. Gregory, U. M. Heller, J. Hetrick, A. S. Kronfeld, P. B. Mackenzie, D. Menscher, M. Nobes, M. Okamoto, M. B. Oktay, J. Osborn, J. Simone, R. Sugar, D. Toussaint, and H. D. Trottier (Fermilab Lattice, MILC, and HPQCD Collaborations), *Phys. Rev. Lett.* **94**, 011601 (2005).
- [56] C. Bernard, C. DeTar, M. Di Pierro, A. X. El-Khadra, R. T. Evans, E. D. Freeland, E. Gamiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, M. Okamoto, J. Simone, R. Sugar, D. Toussaint, and R. S. Van de Water (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **79**, 014506 (2009).
- [57] J. A. Bailey, C. Bernard, C. DeTar, M. Di Pierro, A. X. El-Khadra, R. T. Evans, E. D. Freeland, E. Gamiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, M. Okamoto, J. N. Simone, R. Sugar, D. Toussaint, and R. S. Van de Water (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **79**, 054507 (2009).
- [58] C. Bernard, C. DeTar, M. Di Pierro, A. X. El-Khadra, R. T. Evans, E. D. Freeland, E. Gámiz, S. Gottlieb, U. M. Heller, J. E. Hetrick, A. S. Kronfeld, J. Laiho, L. Levkova, P. B. Mackenzie, J. N. Simone, R. Sugar, D. Toussaint, and R. S. Van de Water (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **83**, 034503 (2011).
- [59] G. P. Lepage, *Phys. Rev. D* **59**, 074502 (1999).
- [60] M. Lüscher and P. Weisz, *Phys. Lett.* **158B**, 250 (1985).
- [61] Z. Hao, G. M. von Hippel, R. R. Horgan, Q. J. Mason, and H. D. Trottier, *Phys. Rev. D* **76**, 034507 (2007).
- [62] K. G. Wilson, in *Quarks and Strings on a Lattice*, edited by A. Zichichi (Plenum, New York, 1975), p. 69.
- [63] M. B. Oktay and A. S. Kronfeld, *Phys. Rev. D* **78**, 014504 (2008).
- [64] H.-W. Lin and N. Christ, *Phys. Rev. D* **76**, 074506 (2007).
- [65] G. P. Lepage, L. Magnea, C. Nakhleh, U. Magnea, and K. Hornbostel, *Phys. Rev. D* **46**, 4052 (1992).
- [66] R. Sommer, *Nucl. Phys.* **B411**, 839 (1994).
- [67] C. W. Bernard, T. Burch, K. Orginos, D. Toussaint, T. A. DeGrand, C. DeTar, S. Gottlieb, U. M. Heller, J. E. Hetrick, and R. Sugar, *Phys. Rev. D* **62**, 034503 (2000).
- [68] C. R. Allton, [arXiv:hep-lat/9610016](#).
- [69] A. Bazavov, W. Freeman, D. Toussaint, C. Bernard, X. Du, J. Laiho, C. DeTar, L. Levkova, M. B. Oktay, S. Gottlieb, U. M. Heller, J. E. Hetrick, J. Osborn, R. Sugar, and R. S. Van de Water (MILC Collaboration), *Proc. Sci.*, CD09 (2009) 007 [[arXiv:0910.2966](#)].
- [70] C. T. H. Davies, E. Follana, I. D. Kendall, G. P. Lepage, and C. McNeile (HPQCD Collaboration), *Phys. Rev. D* **81**, 034506 (2010).
- [71] G. P. Lepage, B. Clark, C. T. H. Davies, K. Hornbostel, P. B. Mackenzie, C. Morningstar, and H. Trottier, *Nucl. Phys. B, Proc. Suppl.* **106-107**, 12 (2002).
- [72] C. Morningstar, *Nucl. Phys. B, Proc. Suppl.* **109**, 185 (2002).
- [73] A. S. Kronfeld, *Nucl. Phys. B, Proc. Suppl.* **53**, 401 (1997).
- [74] N. Kawamoto and J. Smit, *Nucl. Phys. B* **192**, 100 (1981).
- [75] J. L. Richardson, *Phys. Lett.* **82B**, 272 (1979).
- [76] D. P. Menscher, Ph.D. thesis, 2005.
- [77] M. Wingate, J. Shigemitsu, C. T. H. Davies, G. P. Lepage, and H. D. Trottier, *Phys. Rev. D* **67**, 054505 (2003).
- [78] M. D. Pierro and E. Eichten, *Phys. Rev. D* **64**, 114004 (2001).
- [79] G. P. Lepage and P. B. Mackenzie, *Phys. Rev. D* **48**, 2250 (1993).
- [80] Q. Mason, H. D. Trottier, C. T. H. Davies, K. Foley, A. Gray, G. P. Lepage, M. Nobes, and J. Shigemitsu (HPQCD Collaboration), *Phys. Rev. Lett.* **95**, 052002 (2005).
- [81] K. Hornbostel, G. P. Lepage, and C. Morningstar, *Phys. Rev. D* **67**, 034023 (2003).
- [82] D. Arndt and C. J. D. Lin, *Phys. Rev. D* **70**, 014503 (2004).
- [83] C. Bernard (MILC Collaboration), *Phys. Rev. D* **65**, 054031 (2002).
- [84] A. S. Kronfeld and S. M. Ryan, *Phys. Lett. B* **543**, 59 (2002).
- [85] C. G. Boyd and B. Grinstein, *Nucl. Phys.* **B442**, 205 (1995).
- [86] I. W. Stewart, *Nucl. Phys.* **B529**, 62 (1998).
- [87] D. Bećirević, S. Prelovšek, and J. Zupan, *Phys. Rev. D* **68**, 074003 (2003).
- [88] C. Bernard, C. DeTar, S. Gottlieb, U. M. Heller, J. E. Hetrick, L. Levkova, J. Osborn, D. Renner, R. Sugar, and D. Toussaint (MILC Collaboration), *Proc. Sci.*, LATTICE2007 (2007) 090 [[arXiv:0710.1118](#)].
- [89] R. Casalbuoni, A. Deandrea, N. Di Bartolomeo, R. Gatto, F. Feruglio, and G. Nardulli, *Phys. Rep.* **281**, 145 (1997).
- [90] A. Anastassov *et al.* (CLEO Collaboration), *Phys. Rev. D* **65**, 032003 (2002).
- [91] A. Abada, D. Bećirević, Ph. Boucaud, G. Herdoiza, J. P. Leroy, A. Le Yaouanc, O. Pène, and J. Rodriguez-Quintero, *Nucl. Phys. B, Proc. Suppl.* **119**, 641 (2003).
- [92] M. C. Arnesen, B. Grinstein, I. Z. Rothstein, and I. W. Stewart, *Phys. Rev. Lett.* **95**, 071802 (2005).
- [93] H. Ohki, H. Matsufuru, and T. Onogi, *Phys. Rev. D* **77**, 094509 (2008).
- [94] J. Bulava, M. A. Donnellan, and R. Sommer (ALPHA Collaboration), *Proc. Sci.*, LATTICE2010 (2010) 303 [[arXiv:1011.4393](#)].

- [95] C. Aubin, C. Bernard, C.T.H. Davies, C. DeTar, S.A. Gottlieb, A. Gray, E.B. Gregory, J. Hein, U.M. Heller, J.E. Hetrick, G.P. Lepage, Q. Mason, J. Osborn, J. Shigemitsu, R. Sugar, D. Toussaint, H. Trotter, and M. Wingate (HPQCD Collaboration), *Phys. Rev. D* **70**, 031504 (2004).
- [96] C. Bernard, S. Datta, T. DeGrand, C. DeTar, S. Gottlieb, U.M. Heller, C. McNeile, K. Orginos, R. Sugar, and D. Toussaint (MILC Collaboration), *Phys. Rev. D* **66**, 094501 (2002).
- [97] G.P. Lepage, in *From Actions to Answers. Proceedings, Theoretical Advanced Study Institute in Elementary Particle Physics*, edited by T.A. DeGrand and D. Toussaint (World Scientific, Singapore, 1989).
- [98] A. Bazavov, C. Bernard, C. DeTar, X. Du, W. Freeman, S. Gottlieb, U.M. Heller, J.E. Hetrick, J. Laiho, L. Levkova, M.B. Oktay, J. Osborn, R. Sugar, D. Toussaint, and R.S. Van de Water (MILC Collaboration), *Proc. Sci., LATTICE2010* (2010) 074 [[arXiv:1012.0868](https://arxiv.org/abs/1012.0868)].
- [99] C.T.H. Davies, C. McNeile, E. Follana, G.P. Lepage, H. Na, and J. Shigemitsu (HPQCD Collaboration), *Phys. Rev. D* **82**, 114504 (2010).
- [100] P. Dimopoulos, R. Frezzotti, G. Herdoiza, V. Lubicz, C. Michael, D. Palao, G.C. Rossi, F. Sanfilippo, A. Shindler, S. Simula, C. Tarantino, and M. Wagner (ETM Collaboration), *J. High Energy Phys.* **01** (2012) 046.
- [101] B.I. Eisenstein *et al.* (CLEO Collaboration), *Phys. Rev. D* **78**, 052003 (2008).
- [102] J.P. Alexander *et al.* (CLEO Collaboration), *Phys. Rev. D* **79**, 052001 (2009).
- [103] L. Widhalm *et al.* (Belle Collaboration), *Phys. Rev. Lett.* **100**, 241801 (2008).
- [104] P. Naik *et al.* (CLEO Collaboration), *Phys. Rev. D* **80**, 112004 (2009).
- [105] P.U.E. Onyisi *et al.* (CLEO Collaboration), *Phys. Rev. D* **79**, 052002 (2009).
- [106] J.P. Lees *et al.* (BABAR Collaboration), *Phys. Rev. D* **82**, 091103 (2010).
- [107] D. Asner *et al.* (Heavy Flavor Averaging Group), Averages of b -hadron, c -hadron, and τ -lepton Properties, [arXiv:1010.1589](https://arxiv.org/abs/1010.1589), http://www.slac.stanford.edu/xorg/hfag/charm/CHARM10/f_ds/results_20jan11.html, with future updates at <http://www.slac.stanford.edu/xorg/hfag/charm/>.
- [108] E. Gámiz, C.T.H. Davies, G.P. Lepage, J. Shigemitsu, and M. Wingate (HPQCD Collaboration), *Phys. Rev. D* **80**, 014503 (2009).
- [109] C. McNeile, C.T.H. Davies, E. Follana, K. Hornbostel, and G.P. Lepage (HPQCD Collaboration), *Phys. Rev. D* **85**, 031503 (2012).
- [110] C. Albertus, Y. Aoki, P.A. Boyle, N.H. Christ, T.T. Dumitrescu, J.M. Flynn, T. Ishikawa, T. Izubuchi, O. Lektik, C.T. Sachrajda, A. Soni, R.S. Van de Water, J. Wennekers, and O. Witzel (RBC Collaboration and UKQCD Collaboration), *Phys. Rev. D* **82**, 014505 (2010).
- [111] A. Bazavov, C. Bernard, C. DeTar, W. Freeman, S. Gottlieb, U.M. Heller, J.E. Hetrick, J. Laiho, L. Levkova, M. Oktay, J. Osborn, R.L. Sugar, D. Toussaint, and R.S. Van de Water (MILC Collaboration), *Proc. Sci., LATTICE2010* (2010) 320 [[arXiv:1012.1265](https://arxiv.org/abs/1012.1265)].
- [112] E. Follana, C.T.H. Davies, G.P. Lepage, and J. Shigemitsu (HPQCD Collaboration), *Phys. Rev. Lett.* **100**, 062002 (2008).
- [113] B.P.G. Mertens, A.S. Kronfeld, and A.X. El-Khadra, *Phys. Rev. D* **58**, 034505 (1998).

Neutral B -meson mixing from three-flavor lattice quantum chromodynamics: Determination of the $SU(3)$ -breaking ratio ξ

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We study $SU(3)$ -breaking effects in the neutral B_d - $\bar{B}_d$ and B_s - $\bar{B}_s$ systems with unquenched $N_f = 2 + 1$ lattice quantum chromodynamics (QCD). We calculate the relevant matrix elements on the MILC collaboration's gauge configurations with asqtad-improved staggered sea quarks. For the valence light-quarks (u , d , and s) we use the asqtad action, while for b quarks we use the Fermilab action. We obtain $\xi = f_{B_s}\sqrt{B_{B_s}}/f_{B_d}\sqrt{B_{B_d}} = 1.268 \pm 0.063$. We also present results for the ratio of bag parameters B_{B_s}/B_{B_d} and the ratio of Cabibbo-Kobayashi-Maskawa matrix elements $|V_{td}|/|V_{ts}|$. Although we focus on the calculation of ξ , the strategy and techniques described here will be employed in future extended studies of the B mixing parameters $\Delta M_{d,s}$ and $\Delta\Gamma_{d,s}$ in the standard model and beyond.

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I. INTRODUCTION

The observation of new particles at high-energy colliders is not the only way for new physics to be discovered. It can also be unveiled through the observation of deviations from the standard model (SM) via high-precision measurements of low-energy observables in high-luminosity experiments. This requires matching precision in the theoretical SM predictions for these observables. In principle, such a comparison could reveal the exchange of virtual, new heavy particles involving scales much higher than those that can be achieved in direct production at high-energy colliders.

Heavy-flavor physics and, in particular, neutral-meson mixing are potentially very sensitive to these virtual

effects. Neutral-meson mixing occurs at loop level in the SM, see Fig. 1, and it is further suppressed by small Cabibbo-Kobayashi-Maskawa (CKM) matrix elements, so the effect of new particles in the internal loops could be noticeable in the parameters describing the mixing. Indeed, there are several measurements for which there is a $2 - 3\sigma$ difference from the SM prediction. These include $\sin(2\beta)$ [1], the like-sign dimuon charge asymmetry [2], and unitarity triangle (UT) fits [3–7]. It has been argued that these differences may be due to physics beyond the standard model (BSM) affecting the neutral B -meson mixing processes [3,4].

In the B_s^0 system, the relative phase between the decay amplitudes with and without mixing, β_s , could also show BSM effects, as pointed out in Ref. [8] and later hinted at in a Tevatron measurement [9]. Although new measurements at the CDF [10] and D0 detector [11] are in better

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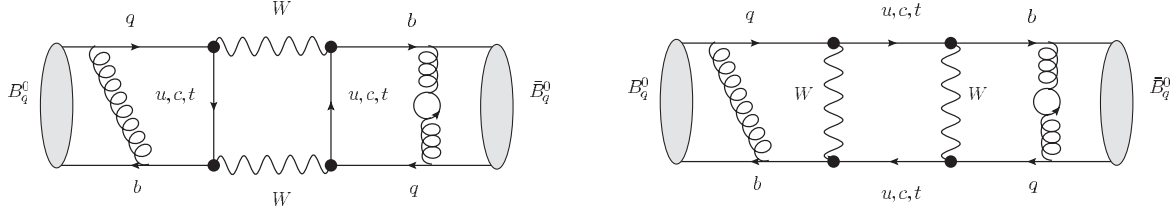


FIG. 1. Box diagrams contributing to $B^0 - \bar{B}^0$ mixing in the SM. Gluon exchanges shown in the plot are just representative of the QCD corrections.

agreement with the SM, reducing the difference from $\sim 3\sigma$ to $\sim 1\sigma$, there is still room for a large deviation of β_s from SM values.

The main parameters describing mixing in the B_s^0 and the B_d^0 systems are the mass differences, $\Delta M_{s(d)}$, and the decay width differences, $\Delta\Gamma_{s(d)}$, between the heavy and light $B_{s(d)}^0$ mass eigenstates, and the CP violating phases $\phi_{s(d)}$. The phases $\phi_{s(d)}$ are defined as the argument of the ratio of the dispersive and absorptive off-diagonal elements of the time evolution matrix which describes the mixing [12]. The existence of new, heavy particles in loops could affect the value of the mass differences, given by the dispersive part of the time evolution matrix. The mass differences ΔM_s [13–15] and ΔM_d [16] have been measured with an accuracy better than 1%. Improving the theoretical control on these quantities is thus crucial in order to fully exploit the potential of CP violating observables to search for nonstandard physics. In addition, the theoretical calculation of BSM contributions to mixing and the experimental measurement of B^0 mixing parameters can help in constraining BSM parameters and understanding new physics [6]. Several recent studies have addressed that task [3–7, 17–24], finding that one of the main limitations to further constraining the parameter space in BSM theories is the error associated with the theoretical calculation of the nonperturbative inputs.

The most interesting quantity to analyze in B^0 mixing phenomena is the $SU(3)$ -breaking ratio ξ , which measures the difference between the mixing parameters in the B_s^0 and the B_d^0 systems, and enters the relation between the ratio of mass differences and CKM matrix elements as

$$\left| \frac{V_{td}}{V_{ts}} \right| = \xi \sqrt{\frac{\Delta M_d M_{B_s}}{\Delta M_s M_{B_d}}}. \quad (1.1)$$

Its value, together with the experimental measurement of the mass differences $\Delta M_{s,d}$, determines the ratio of CKM matrix elements $|V_{td}/V_{ts}|$, which constrains one side of the unitarity triangle [25, 26]. Thus, ξ is one of the key ingredients in UT analyses [3, 5–7].

In the SM, mixing is due to box diagrams with the exchange of two W -bosons, like those in Fig. 1. These box diagrams can be rewritten in terms of an effective Hamiltonian with four-fermion operators describing processes with $\Delta B = 2$. In BSM theories, mixing processes

can receive contributions from additional diagrams due to the exchange of new, heavy particles. These can also be parametrized in terms of four-fermion effective operators built with SM degrees of freedom. The most general effective Hamiltonian describing processes with $\Delta B = 2$ was given in Refs. [27, 28], and can also be found in Ref. [29]. There are a total of five independent operators (plus parity conjugates) in the Hamiltonian, but only three of them contribute to mixing in the SM

$$\mathcal{H}_{\text{eff, SM}}^{\Delta B=2} = \sum_{i=1}^3 C_i \mathcal{O}_i, \quad (1.2)$$

with

$$\begin{aligned} \mathcal{O}_1^q &= (\bar{q}^i \gamma^\nu L b^i)(\bar{q}^j \gamma^\nu L b^j), \\ \mathcal{O}_2^q &= (\bar{q}^i L b^i)(\bar{q}^j L b^j), \\ \mathcal{O}_3^q &= (\bar{q}^i L b^j)(\bar{q}^j L b^i), \end{aligned} \quad (1.3)$$

where i and j are color indices, and L and R are the Dirac projection operators $\frac{1}{2}(1 - \gamma_5)$ and $\frac{1}{2}(1 + \gamma_5)$, respectively. The fields q denote strange or down fields for B_s^0 and B_d^0 mixing, respectively, and b represents the bottom field.

The matrix element of the first operator in Eq. (1.3), $\mathcal{O}_1^q$, provides the mass difference in the SM:

$$\Delta M_q^{\text{SM}} = \frac{G_F^2 M_W^2}{6\pi^2} |V_{tq}^* V_{tb}|^2 \eta_2^B S_0(x_t) M_{B_q} f_{B_q}^2 \hat{B}_{B_q}, \quad (1.4)$$

where $S_0(x_t)$ is the Inami-Lim function [30], which depends on the top quark mass through $x_t = m_t^2/M_W^2$, and the quantity η_2^B is a perturbative quantum chromodynamics correction factor. The products $f_{B_q}^2 \hat{B}_{B_q}$ parametrize the hadronic matrix elements in the effective theory by

$$\langle \bar{B}_q^0 | \mathcal{O}_1^q | B_q^0 \rangle(\mu) = \frac{2}{3} M_{B_q}^2 f_{B_q}^2 \hat{B}_{B_q}(\mu). \quad (1.5)$$

The factors f_{B_q} are the B_q^0 decay constants. The renormalization group invariant bag parameters $\hat{B}_{B_q}$ in Eq. (1.4) are related to the scheme and scale dependent bag parameters in Eq. (1.5) at next-to-leading order (NLO) by

$$\hat{B}_{B_q} = [\alpha_s(\mu)]^{-6/23} \left[1 + \frac{\alpha_s(\mu)}{4\pi} J_5 \right] B_{B_q}(\mu), \quad (1.6)$$

where J_5 is known in both $\overline{\text{MS}}$ -NDR (naive dimensional regularization) and $\overline{\text{MS}}$ -HV ('t Hooft-Veltman) schemes [31]. Bag parameters have traditionally been used to measure the deviation of the four-fermion operator matrix elements from their vacuum insertion values, $B_B = 1$.

The $SU(3)$ -breaking parameter ξ can be written in terms of decay constants and bag parameters

$$\xi = \frac{f_{B_s} \sqrt{B_{B_s}}}{f_{B_d} \sqrt{B_{B_d}}}. \quad (1.7)$$

Many of the uncertainties that affect the theoretical calculation of the decay constants and bag parameters cancel totally or partially in this ratio, leaving the chiral extrapolation as the dominant error. Hence, ξ and the combination of CKM matrix elements related to it, can be determined with a significantly smaller error than the individual matrix elements.

The hadronic matrix elements in Eq. (1.5) encode the nonperturbative physics of the problem and are best calculated using lattice QCD. Our current knowledge of them, limits the accuracy with which the CKM matrix elements appearing in Eq. (1.4) can be determined from the experimental measurements of $\Delta M_{s(d)}$. In particular, the uncertainty associated with the calculation of ξ is one of the main limiting factors in UT analyses, so improvement in the knowledge of ξ is crucial to disentangle the origin of the $2 - 3\sigma$ tension.

There are two $2 + 1$ unquenched lattice calculations of the ratio ξ in the literature. One is by the HPQCD collaboration [32], which quotes the value $\xi = 1.258(33)$. The other is an exploratory study by the RBC and UKQCD collaborations [33] on a single lattice spacing and using the static limit for the bottom quark; their result is $\xi = 1.13(12)$. In this paper, we report a lattice calculation of ξ at the few-percent level.

Preliminary results related to the work here were presented in Refs. [34–37]. In Ref. [34], the simulation and correlator fitting methods were described using data for one lattice spacing, while Refs. [35,36] focused on the discussion of statistical and fitting errors, and the chiral extrapolation method. In Ref. [37], we studied the matching method and the heavy-quark discretization errors.

The primary difference between this work and the HPQCD calculation in Ref. [32] is the treatment of the valence b quarks. The HPQCD collaboration uses lattice NRQCD [38] while we employ the clover action [39] with the Fermilab interpretation [40]. An advantage of the Fermilab method is that it can also be efficiently used to simulate charm quarks, so the analysis performed in this work can be easily extended to the study of the short-distance contributions to D^0 - $\bar{D}^0$ mixing. Although in the case of neutral D mixing the long-distance contributions are believed to be dominant, a calculation of the short-distance contributions can, nevertheless, provide valuable constraints on extensions of the SM [41].

In order to achieve the few-percent level of precision required by phenomenology, we use lattice QCD simulations with realistic sea quarks. In particular, we employ a subset of the magnetic induced laser cooling (MILC) configurations with $2 + 1$ flavors of asqtad sea quarks [42–44]. In the valence sector, we use the same staggered asqtad action to simulate the light quarks. The configurations we use in this analysis were generated using the fourth-root procedure for eliminating extra degrees of freedom originating from fermion doubling. Despite the nonlocal violations of unitarity of the rooted theory at non-zero lattice spacing [45,46], there are strong theoretical arguments [47–50], as well as other analytical and numerical evidence [51–54], that the local, unitary theory of QCD is recovered in the continuum limit. This gives us confidence that the rooting procedure yields valid results. We also explicitly tested the rooting procedure as well as improvements in our heavy action by calculating the spin-dependent hyperfine splittings for B_s and D_s mesons in Ref. [55].

Our collaboration has already successfully used the asqtad MILC ensembles in similar calculations of other quantities involving B mesons, as part of a broad program of calculating matrix elements: for example, the extraction of the CKM matrix elements $|V_{ub}|$ and $|V_{cb}|$ from the calculation of, respectively, the semileptonic form factors describing the processes $B \rightarrow \pi l \nu$ [56] and $B \rightarrow D^* l \nu$ [57,58]; or, more recently, the calculation of the f_B and f_{B_s} decay constants [59] and the form factor ratios between the semileptonic decays $\bar{B} \rightarrow D^+ l^- \bar{\nu}$ and $\bar{B}_s \rightarrow D_s^+ l^- \bar{\nu}$ [60].

This paper is organized as follows. In Sec. II, we describe the actions and parameters used in our numerical simulations, as well as the construction of the mixing operators and correlation functions. Section III presents the renormalization method using one-loop mean field improved lattice perturbation theory. We include a discussion of the errors associated with the matching and numerical values of the matching coefficients used. Next, in Sec. IV, we give the details of the procedure for the correlator fits. Section V is devoted to the chiral-continuum extrapolation, which is performed within the framework of rooted staggered chiral perturbation theory [61–65]. We describe and discuss the choice of the functional form used in the extrapolation, the different fitting methods tested, and the choice of parameters and parametrization. In Sec. VI, we list and estimate the different systematic errors. Finally, Sec. VII compiles our final results for the parameter ξ as well as for $|V_{td}|/|V_{ts}|$, and the ratio of bag parameters B_{B_s}/B_{B_d} . We also discuss planned future improvements in the calculation of B^0 mixing parameters by our collaboration. In Appendix A, we provide the explicit formulas for the chiral fit functions used in the chiral fits described in Sec. V. In Appendix B, we compile the functions needed to estimate the heavy-quark discretization errors in our calculation. Finally, Appendix C

TABLE I. Parameters of the ensembles analyzed in this work. The first two rows show the approximate lattice spacing and the volume. am_l and am_h are the light and strange sea quark masses, respectively. N_{confs} is the number of configurations analyzed from each ensemble, and am_q are the light valence quark masses. The r_1/a values are obtained by fitting the calculated r_1/a to a smooth function [72], as explained in Ref. [66].

$\approx a$ (fm)	$(\frac{L}{a})^3 \times \frac{T}{a}$	am_l/am_h	N_{confs}	am_q	r_1/a
0.12	$24^3 \times 64$	0.005/0.05	529	0.005, 0.007, 0.01, 0.02, 0.03, 0.0415	2.64
0.12	$20^3 \times 64$	0.007/0.05	833	0.005, 0.007, 0.01, 0.02, 0.03, 0.0415	2.63
0.12	$20^3 \times 64$	0.01/0.05	592	0.005, 0.007, 0.01, 0.02, 0.03, 0.0415	2.62
0.12	$20^3 \times 64$	0.02/0.05	460	0.005, 0.007, 0.01, 0.02, 0.03, 0.0415	2.65
0.09	$28^3 \times 96$	0.0062/0.031	557	0.0031, 0.0044, 0.062, 0.0124, 0.0272, 0.031	3.70
0.09	$28^3 \times 96$	0.0124/0.031	534	0.0031, 0.0042, 0.062, 0.0124, 0.0272, 0.031	3.72

discusses our choices for prior central values and widths for the correlator fits.

II. NUMERICAL SIMULATIONS

A. Parameters of the simulations

The $n_f = 2 + 1$ MILC ensembles [66] used in our calculation include the effect of three sea-quark flavors: two degenerate light quarks corresponding to the up and down quarks (although with larger masses than the physical ones), and one heavier quark corresponding to the strange quark. These dynamical quarks are simulated using the asqtad improved staggered action with errors starting at $O(\alpha_s a^2)$ [67]. The gluon action is a Symanzik improved and tadpole improved action, with $O(\alpha_s a^2)$ errors coming from the gluon loops removed [68,69]. The couplings needed to remove the $O(\alpha_s a^2)$ errors coming from quark loops [70] were available only after the generation of configurations was well advanced, so these effects are not accounted for in the MILC ensembles. Thus, the dominant errors in the gauge action are also of $O(a^4, \alpha_s a^2)$.

The valence light-quark propagators are generated using the asqtad action and converted to naive quark propagators using the relation [71]

$$S_{\text{naive}}(x, y) = \Omega(x) \Omega^\dagger(y) S_{\text{staggered}}(x, y), \quad (2.1)$$

where $\Omega(x) = \gamma_0^{x_0} \gamma_1^{x_1} \gamma_2^{x_2} \gamma_3^{x_3}$.

For the heavy bottom quarks we use the Sheikholeslami-Wohlert action [39] with the Fermilab interpretation for heavy-quark systems [40]. This interpretation retains the full mass dependence of the theory within the parameters of the lattice action. A tree-level matching to QCD is then performed via heavy quark effective theory (HQET), after which it can be shown that the errors in the action begin at $O(\alpha_s \Lambda_{\text{QCD}} a, \Lambda_{\text{QCD}}^2 a^2)$ times bounded functions of $m_b a$, the b -quark mass in lattice units.

We perform our analysis at two different values of the lattice spacing, $a \approx 0.12, 0.09$ fm, and for a variety of sea-quark masses. The values used are shown in Table I. The mass of the heavy b quark is fixed to its physical value by computing the spin-averaged B_s kinetic mass [55]. This determines the b quark's hopping parameters, $\kappa_b = 0.0860$

for the $a \approx 0.12$ fm lattice and $\kappa_b = 0.0923$ for the $a \approx 0.09$ fm lattice [55], and thus the bare b quark mass. We simulate the B mesons with the six different values of light-valence quark mass listed in Table I, the smallest of which is around $m_s/8$, in order to facilitate the extrapolation/interpolation to the physical down/strange quark masses.

B. Correlators: The open-meson propagator

As described in the introduction, the study of the $SU(3)$ -breaking ratio ξ requires the calculation of the hadronic matrix elements¹ $\langle \mathcal{O}_1^q \rangle$ and $\langle \mathcal{O}_2^q \rangle$, the latter of which mixes with $\langle \mathcal{O}_1^q \rangle$ under renormalization, for both $q = d, s$. The matrix elements are obtained from three-point correlation functions with zero spatial momentum

$$C_{\mathcal{O}_i^q}(t_x, t_y) = \sum_{\mathbf{x}, \mathbf{y}} \langle \bar{B}_q^0(t_y, \mathbf{y}) \mathcal{O}_i^q(0) B_q^0(t_x, \mathbf{x})^\dagger \rangle, \quad (2.2)$$

where $i = 1$ or 2 , and the B -meson creation operator $B_q^0(t, \mathbf{x})^\dagger = \sum_{\mathbf{x}'} \bar{b}(t, \mathbf{x}') S(\mathbf{x}, \mathbf{x}') \gamma_5 q(t, \mathbf{x})$, with $q(t, \mathbf{x})$ the naive light quark field, whose propagator is constructed from the staggered propagator *via* Eq. (2.1), and with $S(\mathbf{x}, \mathbf{x}')$ a smearing function. Our choice of smearing function is discussed in Sec. . The structure of the functions in Eq. (2.2) is depicted in Fig. 2. The four-fermion operators $\mathcal{O}_i^q$ are placed at the origin while B -mesons are positioned at x and y . This layout allows us to perform the three-point function fits over both t_x and t_y , maximizing the information included in the fits. In order to extract the relevant matrix elements from Eq. (2.2), we need to determine the overlap of the B -meson creation operator with the ground state. Therefore, we also need the pseudoscalar two-point correlator with zero spatial momentum

$$C_{\text{PS}}(t) = \sum_{\mathbf{x}} \langle \bar{B}_q^0(t, \mathbf{x}) B_q^0(0, 0)^\dagger \rangle. \quad (2.3)$$

The calculation of both three-point and two-point correlators can be organized into convenient structures. Starting with a general correlator with Dirac structure $\Gamma_1 \times \Gamma_2$,

¹To simplify the notation, we define $\langle \mathcal{O}_i^q \rangle \equiv \langle \bar{B}_q^0 | \mathcal{O}_i^q | B_q^0 \rangle$ for $i = 1, 2$.

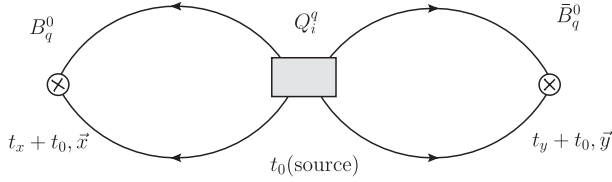


FIG. 2. Structure of the three-point correlators. A B_q^0 is created at rest at $t_x + t_0 < t_0$. At time t_0 , it oscillates into a $\bar{B}_q^0$ via the operator $\mathcal{O}_i^q$, which is subsequently annihilated at $t_y + t_0 > t_0$.

which accommodates a full set of $\Delta B = 2$ four-quark operators, including those in Eq. (1.3),

$$C_3(t_x, t_y) = \sum_{x,y} \langle \bar{B}_q^0(t_y, y) \bar{q}(0) \Gamma_1 b(0) \bar{q}(0) \Gamma_2 b(0) B_q^0(t_x, x)^\dagger \rangle, \quad (2.4)$$

and performing the four possible Wick contractions, we obtain

$$\begin{aligned} C_3(t_x, t_y) &= \sum_{x,y} \{ \text{tr}[\gamma_5 L_q(x, 0) \Gamma_1 H_b(0, x)] \text{tr}[\gamma_5 L_q(y, 0) \Gamma_2 H_b(0, y)] \\ &\quad + \text{tr}[\gamma_5 L_q(y, 0) \Gamma_1 H_b(0, y)] \text{tr}[\gamma_5 L_q(x, 0) \Gamma_2 H_b(0, x)] \\ &\quad - \text{tr}[\gamma_5 L_q(x, 0) \Gamma_1 H_b(0, y) \gamma_5 L_q(y, 0) \Gamma_2 H_b(0, x)] \\ &\quad - \text{tr}[\gamma_5 L_q(x, 0) \Gamma_2 H_b(0, y) \gamma_5 L_q(y, 0) \Gamma_1 H_b(0, x)] \} \end{aligned} \quad (2.5)$$

$$\begin{aligned} &= \sum_{x,y} \{ \text{tr}[L_q(x, 0) \Gamma_1 \gamma_5 H_b^\dagger(x, 0)] \text{tr}[L_q(y, 0) \Gamma_2 \gamma_5 H_b^\dagger(y, 0)] \\ &\quad + \text{tr}[L_q(y, 0) \Gamma_1 \gamma_5 H_b^\dagger(y, 0)] \text{tr}[L_q(x, 0) \Gamma_2 \gamma_5 H_b^\dagger(x, 0)] \\ &\quad - \text{tr}[L_q(x, 0) \Gamma_1 \gamma_5 H_b^\dagger(y, 0) L_q(y, 0) \Gamma_2 \gamma_5 H_b^\dagger(x, 0)] \\ &\quad - \text{tr}[L_q(x, 0) \Gamma_2 \gamma_5 H_b^\dagger(y, 0) L_q(y, 0) \Gamma_1 \gamma_5 H_b^\dagger(x, 0)] \}, \end{aligned} \quad (2.6)$$

$$\begin{aligned} &- \text{tr}[L_q(x, 0) \Gamma_1 \gamma_5 H_b^\dagger(y, 0) L_q(y, 0) \Gamma_2 \gamma_5 H_b^\dagger(x, 0)] \\ &- \text{tr}[L_q(x, 0) \Gamma_2 \gamma_5 H_b^\dagger(y, 0) L_q(y, 0) \Gamma_1 \gamma_5 H_b^\dagger(x, 0)], \end{aligned} \quad (2.7)$$

where L_q is the (naive) light-quark propagator, and H_b is the heavy-quark propagator. The traces in Eq. (2.5) run over spin and color indices.

These correlators can be rewritten as

$$\begin{aligned} C_3(t_x, t_y) &= \Gamma_1^{\beta\alpha} E_{aa}^{\alpha\beta}(t_x) \Gamma_2^{\sigma\tau} E_{cc}^{\sigma\tau}(t_y) \\ &\quad + \Gamma_1^{\beta\alpha} E_{aa}^{\alpha\beta}(t_y) \Gamma_2^{\tau\sigma} E_{cc}^{\sigma\tau}(t_x) \\ &\quad - \Gamma_1^{\beta\alpha} E_{ac}^{\alpha\sigma}(t_x) \Gamma_2^{\sigma\tau} E_{ca}^{\tau\beta}(t_y) \\ &\quad - \Gamma_1^{\beta\alpha} E_{ac}^{\alpha\sigma}(t_y) \Gamma_2^{\tau\sigma} E_{ca}^{\tau\beta}(t_x), \end{aligned} \quad (2.8)$$

where summation over repeated indices is implied, and we have introduced the basic objects

$$E_{ac}^{\alpha\beta}(t) = \gamma_5^{\alpha\sigma} H_{b,da}^{*\tau\sigma}(t, 0) L_{q,dc}^{\tau\beta}(t, 0), \quad (2.9)$$

with Dirac indices labeled as $\alpha, \beta, \sigma, \tau$ and color indices labeled as a, c, d . We call the combination of propagators $E_{ad}^{\alpha\beta}(t_x)$ defined in Eq. (2.9) “open-meson propagator”. Once the open-meson propagators have been computed and saved, all correlation functions needed for B -meson mixing, including BSM operators, can be immediately constructed by contracting them with the appropriate Dirac structures. As shown in Eq. (2.8), the three-point correlators are obtained by combining two open-meson propagators, while for the two-point correlators we only need one open-meson propagator.

C. Doubler modes' effect on the correlation functions

The remnant doubling degeneracy of staggered fermions leads to contributions of scalar states, in addition to pseudoscalar states, in correlation functions with external pseudoscalar particles. The scalar contamination yields oscillating terms in the correlation functions [71]. In this section, we extend the analysis of Ref. [71] for two-point correlation functions, to the three-point functions introduced in Sec. II B. We conclude that the effect of the doubler modes on the three-point functions can be removed at leading order in the lattice spacing through appropriate fits of the Euclidean time-dependence.

The *doubling* symmetry of the original naive action under the transformation

$$\psi(x) \rightarrow e^{ix \cdot \pi_g} M_g \psi(x), \quad \bar{\psi}(x) \rightarrow e^{ix \cdot \pi_g} \bar{\psi}(x) M_g^\dagger, \quad (2.10)$$

where

$$M_g = \prod_{\mu \in g} i\gamma_5 \gamma_\mu, \quad (2.11)$$

$$G = \{g: g = (\mu_1, \mu_2, \dots), \mu_1 < \mu_2 < \dots\}, \quad (2.12)$$

$$(\pi_g)_\mu = \begin{cases} \frac{\pi}{a} & \text{if } \mu \in g \\ 0 & \text{otherwise} \end{cases} \quad (2.13)$$

generates sixteen equivalent species of quarks, referred to as *tastes*, that can be reduced to four by staggering the quark field [73]. Each element of G is a list of up to four indices, e.g., (2), (0,3), and (0,1,2,3) are elements of G , as is the empty set $\emptyset$. Different g 's label different doubler modes, or tastes.

Consider the general three-point function in momentum space,

$$\begin{aligned}
C_{\Gamma_1 \times \Gamma_2}(t_x, t_y) &= \sum_{x,y} \langle \bar{b}(x) \gamma_5 q(x) [\bar{q}(0) \Gamma_1 b(0) \bar{q}(0) \Gamma_2 b(0)] \bar{b}(y) \gamma_5 q(y) \rangle \\
&= \int_{-\pi/a}^{\pi/a} \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{d^3 \mathbf{k}}{(2\pi)^3} \langle \bar{b}(\mathbf{p}, t_x) \gamma_5 \tilde{q}(\mathbf{p}, t_x) \\
&\quad \times [\bar{q}(0) \Gamma_1 b(0) \bar{q}(0) \Gamma_2 b(0)] \bar{b}(\mathbf{k}, t_y) \gamma_5 \tilde{q}(\mathbf{k}, t_y) \rangle, \quad (2.14)
\end{aligned}$$

where $\Gamma_1 \times \Gamma_2$ denotes the Dirac structure of the four-fermion operators in Eq. (1.3). For simplicity of notation, we omit the smearing function from the B -meson operator and write it as $\bar{b}(x) \gamma_5 q(x)$. It would be straightforward (but not particularly instructive) to generalize the expressions of Eqs. (2.14), (2.15), (2.16), (2.17), (2.18), (2.19), and (2.20) to include the smearing function.

For now the bracketed four-quark operator is left in position space and $\tilde{b}$, $\tilde{q}$ are the spatial momentum-space bottom and strange/down fermion fields. Because of the

doubling symmetry, we can integrate over the central half of the Brillouin zone and sum over the spatial doublers

$$\begin{aligned}
C_{\Gamma_1 \times \Gamma_2}(t_x, t_y) &= \sum_{g_s, g'_s} \int_{-\pi/2a}^{\pi/2a} \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{d^3 \mathbf{k}}{(2\pi)^3} \\
&\quad \times \langle \bar{b}(\mathbf{p} + \pi_{g_s}, t_x) \gamma_5 \tilde{q}(\mathbf{p} + \pi_{g_s}, t_x) \\
&\quad \times [\bar{q}(0) \Gamma_1 b(0) \bar{q}(0) \Gamma_2 b(0)] \\
&\quad \times \bar{b}(\mathbf{k} + \pi_{g'_s}, t_y) \gamma_5 \tilde{q}(\mathbf{k} + \pi_{g'_s}, t_y) \rangle, \quad (2.15)
\end{aligned}$$

where g_s denotes a particular spatial doubler mode. Due to the high momentum that is imparted to the heavy quark when $g_s \neq \emptyset$, such states are far off shell and have a negligible effect on the correlation function. The taste of the temporal modes can now be considered by Fourier transforming the light quarks' temporal component, and then again restricting the Brillouin zone and summing over the doublers

$$\begin{aligned}
C_{\Gamma_1 \times \Gamma_2}(t_x, t_y) &= \int_{-\pi/2a}^{\pi/2a} \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{d^3 \mathbf{k}}{(2\pi)^3} \int_{-\pi/2a}^{\pi/2a} \frac{dp_0}{(2\pi)} \frac{dk_0}{(2\pi)} e^{ip_0 t_x + ik_0 t_y} \langle \bar{b}(\mathbf{p}, t_x) \gamma_5 [\tilde{q}'(\mathbf{p}, p_0) + (-1)^{t_x} \tilde{q}'(\mathbf{p}, p_0 + \pi/a)] \\
&\quad \times [\bar{q}(0) \Gamma_1 b(0) \bar{q}(0) \Gamma_2 b(0)] \bar{b}(\mathbf{k}, t_y) \gamma_5 [\tilde{q}'(\mathbf{k}, k_0) + (-1)^{t_y} \tilde{q}'(\mathbf{k}, k_0 + \pi/a)] \rangle. \quad (2.16)
\end{aligned}$$

With the momentum space spinors $\tilde{f}^{\text{rs}}$ defined as

$$\tilde{f}^{\text{rs}}(p) = \prod_{\mu \in g} i \gamma_5 \gamma_\mu \tilde{q}'(p + \pi_g), \quad (2.17)$$

so that

$$\tilde{q}'(\mathbf{p}, p_0) = \tilde{f}'(\mathbf{p}, p_0), \quad \tilde{q}'(\mathbf{p}, p_0 + \pi/a) = i \gamma_5 \gamma_0 \tilde{f}'^0(\mathbf{p}, p_0), \quad (2.18)$$

the three-point function can be written as

$$\begin{aligned}
C_{\Gamma_1 \times \Gamma_2}(t_x, t_y) &= \int_{-\pi/2a}^{\pi/2a} \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{d^3 \mathbf{k}}{(2\pi)^3} \langle \bar{b}(\mathbf{p}, t_x) \gamma_5 [\tilde{f}(\mathbf{p}, t_x) + (-1)^{t_x} i \gamma_5 \gamma_0 \tilde{f}^0(\mathbf{p}, t_x)] [\bar{q}(0) \Gamma_1 b(0) \bar{q}(0) \Gamma_2 b(0)] \\
&\quad \times \bar{b}(\mathbf{k}, t_y) \gamma_5 [\tilde{f}(\mathbf{k}, t_y) + (-1)^{t_y} i \gamma_5 \gamma_0 \tilde{f}^0(\mathbf{k}, t_y)] \rangle, \quad (2.19)
\end{aligned}$$

where the superscript 0 indicates a temporal taste and no superscript is the null taste at the center of the Brillouin zone.

After Fourier transforming, the bracketed four-quark operator has no restrictions on the tastes that contribute to it. However, it must be contracted with the external quark fields to form the propagators. Because the asqtad action is used, contractions between tastes of different types are suppressed to $O(a^2 \alpha_s^2)$. The three-point function then takes the form

$$\begin{aligned}
C_{\Gamma_1 \times \Gamma_2}(t_x, t_y) &= \int_{-\pi/2a}^{\pi/2a} \frac{d^3 \mathbf{p}}{(2\pi)^3} \frac{d^3 \mathbf{k}}{(2\pi)^3} \langle \bar{b}(\mathbf{p}, t_x) \gamma_5 [f(\mathbf{p}, t_x) + (-1)^{t_x} i \gamma_5 \gamma_0 f^0(\mathbf{p}, t_x)] \\
&\quad \times [(\bar{f}(0) + i \gamma_5 \gamma_0 \bar{f}^0(0)) \Gamma_1 b(0) (\bar{f}(0) + i \gamma_5 \gamma_0 \bar{f}^0(0)) \Gamma_2 b(0)] \bar{b}(\mathbf{k}, t_y) \gamma_5 [f(\mathbf{k}, t_y) + (-1)^{t_y} i \gamma_5 \gamma_0 f^0(\mathbf{k}, t_y)] \rangle, \quad (2.20)
\end{aligned}$$

where higher order terms coming from contractions between quarks of different taste give terms of $O(a^2 \alpha_s^2)$ that are not considered here. The effects of such terms are comparable to NLO terms in staggered chiral perturbation theory and need to be considered at that order. They give rise to the “wrong spin” terms discussed below. According to Eq. (2.20), the leading-order correlation functions have

contributions from both the pseudoscalar and the scalar states. The latter ones are known as oscillating states, since the sign of their contribution oscillates with time.

The fit ansatz for our correlators must model both regular and oscillating contributions, so that we can remove the latter and extract the physical matrix elements. This is done using the form

$$C_{O_i^q}(t_x, t_y) = \sum_{\alpha, \beta=0}^{N_{\text{states}}-1} Z_\alpha Z_\beta \frac{O_{\alpha\beta}^i}{\sqrt{2E_\alpha 2E_\beta}} \times (-1)^{(t_x+1)\alpha+(t_y+1)\beta} e^{-E_\alpha t_x - E_\beta t_y}, \quad (2.21)$$

where the sum is over a finite number of states N_{states} . The time t_x in Eq. (2.21) and in the discussion on fitting in Sec. IV is the number of time slices between the initial state and the operator, and thus it is a positive number, unlike the time t_x defined in Fig. 2. The oscillations in Euclidean time given by the factor $(-1)^{(t_x+1)\alpha+(t_y+1)\beta}$ reflect the contribution from the scalar states in Eq. (2.20). The matrix elements of interest are given by the three-point amplitude of the ground state $\alpha = \beta = 0$, O_{00}^i . Analogously, we incorporate regular and oscillating contributions to the description of the two-point correlators by using the following functional form in the fits

$$C_{\text{PS}}(t) = \sum_{\alpha=0}^{N_{\text{states}}-1} |Z_\alpha|^2 (-1)^{(t+1)\alpha} (e^{-E_\alpha t} + e^{-E_\alpha(T-t)}), \quad (2.22)$$

where T is the temporal size of the lattice. Three- and two-point functions are fit simultaneously in our analysis, as described in Sec. IV.

D. Improving the heavy-light four-quark operator

In addition to the discretization errors in the heavy-quark action, the mixing operator also has discretization errors due to the difference in the small-momentum behavior of lattice and continuum heavy quarks. In this section,

we describe how the lowest order of operator discretization errors are removed in our calculation. We first show that the errors start at $O(ap)$ and then discuss how the error at this order can be removed by a “rotation” of the heavy-quark field.

To begin, consider the small ap expansion of the spinor for the Wilson-like fermion

$$u^{\text{lat}}(\chi, p) = \frac{\gamma_0 \text{sign} \chi \sinh Ea - i \gamma_j \sin(p_j a) + L}{\sqrt{2L(L + \sinh Ea)}} u(\chi, 0) \\ = e^{-m_1 a/2} \left[1 - \frac{i \gamma \cdot p a}{2 \sinh m_1 a} + O((ap)^2) \right] u(\chi, 0), \quad (2.23)$$

where χ labels spin and particle vs antiparticle, $\hat{p} = (2/a) \sin(pa/2)$, and for the clover action $L = 1 + m_0 a + \frac{1}{2} \hat{p}^2 a^2 - \cos p_0 a$. The continuum spinor has the expansion

$$u^{\text{cont}}(\chi, p) = \left[1 - \frac{i \gamma \cdot p}{2m} + O((ap)^2) \right] u(\chi, 0). \quad (2.24)$$

The mismatch between the small-momentum terms can be easily removed by “rotating” the lattice heavy quark as was done to heavy-light bilinear operators in Ref. [40]. The light lattice spinors for the staggered formulation have the same small-momentum behavior as in the continuum up to $O((pa)^2, (m_q a)^2)$ and need not be matched.

The analysis of Ref. [40] can be generalized from bilinears to four-fermion operators with Dirac structure $\Gamma_1 \times \Gamma_2$. We can take one of the terms in the contraction of the lattice operator

$$\langle q(p'_q), b(p'_b) | \bar{q} \Gamma_1 b \bar{q} \Gamma_2 b | q(p_q), b(p_b) \rangle_{\text{lat}} = N_q(p'_q) N_q(p_q) N_b(p'_b) N_b(p_b) \bar{u}(p'_q) \Gamma_1 u_h^{\text{lat}}(p'_b) \bar{u}(p_q) \Gamma_2 u_h^{\text{lat}}(p_b) \\ + (\text{additional contractions}), \quad (2.25)$$

where $N_q(p)$ and $N_b(p)$ are normalization factors for the q and b one-particle states. Following the Fermilab interpretation in Ref. [40], we demand that lattice and continuum amplitudes match through $O(ap)$,

$$Z \left(\bar{u}(\chi, p'_q) \Gamma_1 e^{-am_1^b/2} \left[1 - \frac{i \gamma \cdot p'_b a}{2 \sinh am_1^b} \right] u(\chi, 0) \bar{u}(\chi, p_q) \Gamma_2 e^{-am_1^b/2} \left[1 - \frac{i \gamma \cdot p_b a}{2 \sinh am_1^b} \right] u(\chi, 0) \right) + a Z D_n Q_n \\ = \bar{u}(\chi, p'_q) \Gamma_1 \left[1 - \frac{i \gamma \cdot p'_b}{2m_b} \right] u(\chi, 0) \times \bar{u}(\chi, p_q) \Gamma_2 \left[1 - \frac{i \gamma \cdot p_b}{2m_b} \right] u(\chi, 0) + O((pa)^2), \quad (2.26)$$

where Q_n are dimension-seven lattice operators and D_n their corresponding coefficients. These operators and coefficients are straightforward to identify (m_b must be identified with the Fermilab kinetic mass, M_2 [74]). There are two dimension-seven operators contributing to the matching, $Q_1 = \bar{q} \Gamma_1 \gamma \cdot D b \bar{q} \Gamma_2 b$ and $Q_2 = \bar{q} \Gamma_1 b \bar{q} \Gamma_2 \gamma \cdot D b$, which will remove the pa discrepancy for appropriate values of the Wilson coefficients and the normalization constant. From the relation above, we find

$$D_1 = D_2 = \left[\frac{1}{\sinh am_1^b} - \frac{1}{2am_2^b} \right] \quad (2.27)$$

and

$$Z = e^{am_1^b}. \quad (2.28)$$

Here, m_1 and m_2 are again the Fermilab rest and kinetic masses defined in Ref. [40].

However, through $O(ap)$, adding these operators has the same effect as inducing a “rotation” of the heavy field

$$b^r(x) = [1 + ad_1 \boldsymbol{\gamma} \cdot \mathbf{D}]b(x), \quad (2.29)$$

where

$$d_1 = D_1 = D_2. \quad (2.30)$$

This removes $O(\Lambda_{\text{QCD}}a)$ discretization errors in the operator. The leading errors are then $O((\Lambda_{\text{QCD}}a)^2)$ and $O(\alpha_s \Lambda_{\text{QCD}}a)$. In the way we have set up the calculation, the open-meson propagators, Eq. (2.9), include the rotation.

III. MATCHING OF THE LATTICE MATRIX ELEMENTS

In order to cancel the scheme and scale dependence of the Wilson coefficients in the effective Hamiltonian, we must relate the bare hadronic matrix elements of the lattice operators in Eq. (1.3) to a continuum scheme. We perform that renormalization and matching perturbatively at one-loop. In the lattice part of this renormalization calculation we use mean field improved lattice perturbation theory [75] to improve the convergence of the theory by resumming the tadpole contributions.

Already at one-loop, even in the continuum, the operators in Eq. (1.3) mix with each other under renormalization. To extract the renormalized value of $\langle \mathcal{O}_1^q \rangle$, we use the following matching relation

$$\begin{aligned} \langle \mathcal{O}_1^q \rangle^{\text{renor}}(\mu) = & \mathcal{C} \{ [1 + \alpha_s \cdot \zeta_{11}(\mu, m_b, am_b)] \langle \mathcal{O}_1^q \rangle^{\text{lat}} \\ & + \alpha_s \cdot \zeta_{12}(\mu, m_b, am_b) \langle \mathcal{O}_2^q \rangle^{\text{lat}} \} \\ & + O(\alpha_s^2, \alpha_s \Lambda_{\text{QCD}}a), \end{aligned} \quad (3.1)$$

where the renormalization coefficients ζ_{ij} are the difference between the renormalizations in the continuum and on the lattice, $\zeta_{ij} = Z_{ij}^{\text{cont}} - Z_{ij}^{\text{lat}}$. The continuum renormalization scale at which we perform the matching is μ . The lattice spacing is a and $\mathcal{C}$ is a factor which absorbs the lattice field normalization conventions. The values of Z_{ij}^{cont} are listed in Ref. [76] and a detailed description of the calculation of the lattice renormalization coefficients will be given in Ref. [77]. Table II lists the tadpole-improved renormalization coefficients relevant for the lattice data analyzed in this paper. For each lattice spacing and b quark mass we show the infrared (IR) finite part of the Z_{ij}^{lat} 's as

TABLE II. Values of the finite part of the lattice one-loop renormalization coefficients Z_{ij}^{lat} , the difference of the continuum and lattice one-loop coefficients ζ_{ij} needed in Eq. (3.1) for the 0.12 fm and 0.09 fm lattices, and the coupling α_s used in the matching relation. The continuum ($\overline{\text{MS}}$ -NDR) scale used in the matching is $\mu = m_b$.

$\approx a$ (fm)	am_b	$Z_{11}^{\text{lat,finite}}$	$Z_{12}^{\text{lat,finite}}$	$\zeta_{11}^{\overline{\text{MS}}\text{-NDR}}$	$\zeta_{12}^{\overline{\text{MS}}\text{-NDR}}$	α_s
0.12	2.1881	-0.726	-0.325	0.1998	-0.312	0.32
0.09	1.7728	-0.945	-0.369	0.3041	-0.268	0.26

well as the corresponding ζ_{ij} (in the $\overline{\text{MS}}$ -NDR continuum scheme). The ζ_{ij} are IR finite since the IR divergent contributions to Z_{ij}^{lat} and Z_{ij}^{cont} cancel in the difference. All the coefficients Z_{ij}^{lat} in Table II are between 0.3 and 1, which indicates a sensible behavior of the lattice perturbation series.

In order to apply the matching relation Eq. (3.1), we need to choose both a scale μ and a value for the strong coupling constant α_s . For the scale, we use the bottom quark mass and, in that way, eliminate higher-order logarithmic contributions that come in powers of $\log(\mu/m_b)$. For the strong coupling constant, we use the renormalized coupling in the V -scheme [69] evaluated at a scale q^* , as in Ref. [78]. The scale q^* should be the size of a typical gluon loop momentum in this process and can be calculated using the methods outlined in Refs. [69,79]. Here, we use $q^* = 2/a$ which is close to the calculated value for heavy-light currents using the same actions we are employing [69,80]. This is justified since the contributions coming from the current renormalization are larger than the intrinsic four-quark contributions [77]. The values of α_V are determined from the static-quark potential in a manner similar to that described in Ref. [78] and are also given in Table II.

IV. FITTING METHOD AND STATISTICAL ERRORS

The correlation functions are calculated at four different time sources t , and then averaged over time sources. For the $a \approx 0.12$ fm ensembles, $t_0 = 0, 16, 32, 48$, and for the $a \approx 0.09$ fm ensembles, $t_0 = 0, 24, 48, 72$. The statistical errors in the data and fits decrease with each additional time source by approximately what is expected, suggesting that the correlators from different time sources are weakly correlated and statistical power is gained by averaging.

In order to extract the renormalized matrix elements, we tried two methods for the correlator fits. In the first method, we fit the bare correlators and combine the results afterwards with the matching coefficients in Sec. III to get the renormalized matrix elements. In the second method, we first apply the matching coefficients to the correlators for each configuration and then perform the fits to obtain the renormalized matrix elements. The central values are nearly identical with both methods, but the errors are slightly better and the fits more stable with the latter, so for the rest of this article we discuss only the results obtained with the second method.

A. Description of the fitting method and stability tests

The heavy quark in the two-point and three-point correlation functions is always rotated at the source as explained in Sec. II D. For three-point functions, we smear the heavy quarks at the sink using a function based on the quarkonium 1S wave function [81,82]. For two-point functions, at the sink we either rotate local heavy quarks, or we smear

them with a 1S wave function. Smearing greatly improves the overlap with the ground state. The additional rotation at the sink is to ensure that the local-local meson correlator is positive-definite. The naive light-quark propagator is always local at source and sink.

The two-point and three-point correlators used to determine the matrix element $\langle \mathcal{O}_1^q \rangle$ on a particular ensemble and for a particular choice of valence-mass m_q are fit simultaneously using the Bayesian fitting approach described in Refs. [83,84]. For the matrix elements on the coarse ensembles, we find the smallest errors and greatest stability using three correlators (two two-point correlation functions and one three-point correlation function):

- (i) C_{PS} in Eq. (2.22) with local source and local sink.
- (ii) C_{PS} with local source and 1S smeared sink.
- (iii) $C_{\mathcal{O}_1^q}$ in Eq. (2.21) with local source and 1S smeared sink.

For the fine ensembles, the best results are obtained with only one two-point function and one three-point function:

- (i) C_{PS} with 1S smeared source and 1S smeared sink.
- (ii) $C_{\mathcal{O}_1^q}$ with local source and 1S smeared sink.

The prior central values function as the initial starting guesses for our fits. Hence, we choose ground-state values guided by our data to help the fits converge. The prior central values for the ground-state masses are obtained from effective mass plots. For the overlap factors Z_0^d and Z_0^{1S} , where superscripts d and 1S denote factors corresponding to local or 1S smeared sources/sinks, we examine the amplitude of the B -meson propagator with the exponential of the ground state removed. We do the same for O_{00} , where the Z_0^{1S} amplitudes are accounted for. The prior widths are taken to be large compared with the statistical error of the parameters as reported by the fitter to avoid influencing our fit results by our choice of priors. For the higher states' overlap factors, the prior width is chosen based on the expectation that the overlaps should not be larger than the corresponding ground state ones. The energy differences have prior central values and widths that allow them to vary from $\Delta E_{i+1,i} \equiv a(E_{i+1} - E_i) \approx 0.14\text{--}0.37$, where experimental values [16] have been used as a guide. We checked that the prior widths for all fitting parameters are large enough so they do not influence the central value of relevant quantities extracted from the fits.

The same priors are used for all ensembles, except for the masses of the regular and oscillating ground states, E_0 and E'_0 , respectively. These parameters are strongly determined by the data, and very different at each lattice spacing, therefore the prior choice must also be lattice-spacing dependent. Appendix C contains a list of the prior central values and widths we use in the calculation.

Statistical errors are estimated with the bootstrap method. Specifically, for each ensemble and valence mass, 500 bootstrap ensembles are constructed from the

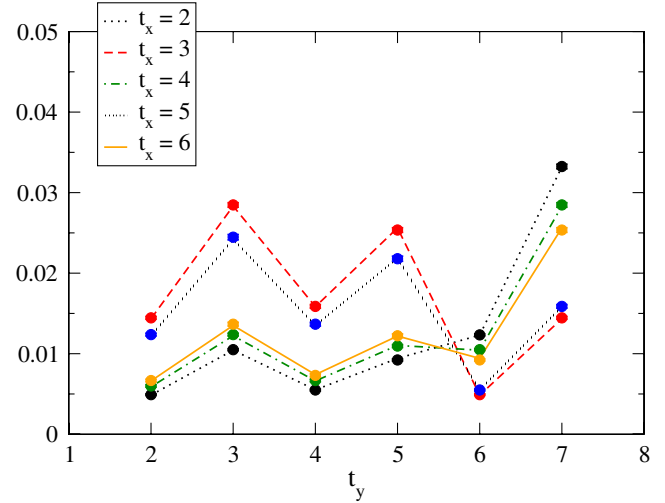


FIG. 3 (color online). Comparison of a fit with correlator data for the correlation function $C_{\mathcal{O}_1^q}(t_x, t_y)$ at fixed $t_x = 2\text{--}6$ (labeled by line type) and as a function of t_y , for the $a \approx 0.09$ fm ensemble with quark masses 0.0124/0.031 and valence quark mass $am_q = 0.031$. The lines connect the fit function results for integer values of t_x, t_y coming from the same single fit and evaluated at specific t_x , and the dots are the average over simulation data. Statistical errors on the simulation data are smaller than the plot symbols. The fit results describe very well the oscillation in time shown by the data.

original ensemble by sampling with replacement. A fit is then performed to each ensemble. We find that, as long as the bootstrap ensembles are larger than ~ 100 , the estimated error is independent of bootstrap ensemble size. For fitting methodology checks and plotting purposes in Figs. 3–6, statistical errors in the parameters are estimated by the average 68% bootstrap error, which is defined as half of the distance between the two points at which 16% of the distribution has a higher (lower) value.

Autocorrelations necessarily exist between correlation functions calculated on different configurations within an ensemble and can be minimized by binning the data. The autocorrelations are observable only in a few ensembles and valence masses. In many ensembles and mass combinations, the noise is large enough that the autocorrelations are not observable. We choose a conservative bin size of 4.

The number of states included in the sum in Eq. (2.21) and the time ranges we use in the fits are shown in Table III. The minimum time slice is fixed to be the same for all the correlators in the fit, three-point as well as two-point. However, the maximum time is fixed separately for the two- and three-point functions. Following Ref. [83], the number of states are determined by first performing the fit using $1 + 1$ states (1 regular state + 1 oscillatory state) starting at large time slices, where the higher-energy states no longer contribute significantly and a good χ^2 per degree of freedom (d.o.f.) is obtained (≈ 1). The fit is then performed using one lower time slice as the starting time

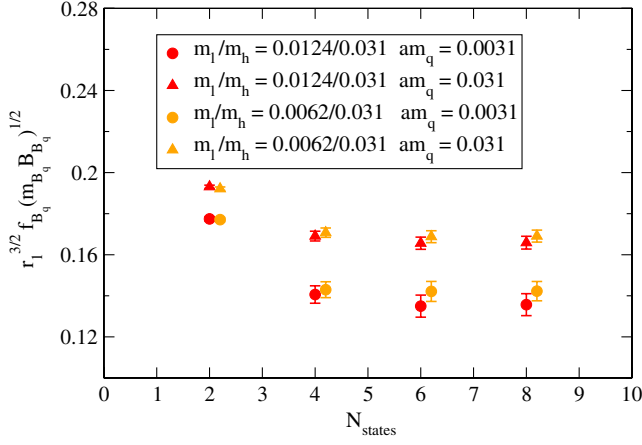


FIG. 4 (color online). $r_1^{3/2} f_{B_q} \sqrt{M_{B_q} B_{B_q}}$ for the two $a \approx 0.09$ fm ensembles for $am_q = 0.031, 0.0031$ as a function of the number of states N_{states} . The fit results for $f_{B_q} \sqrt{M_{B_q} B_{B_q}}$ reach a plateau for $N_{\text{states}} \geq 4$.

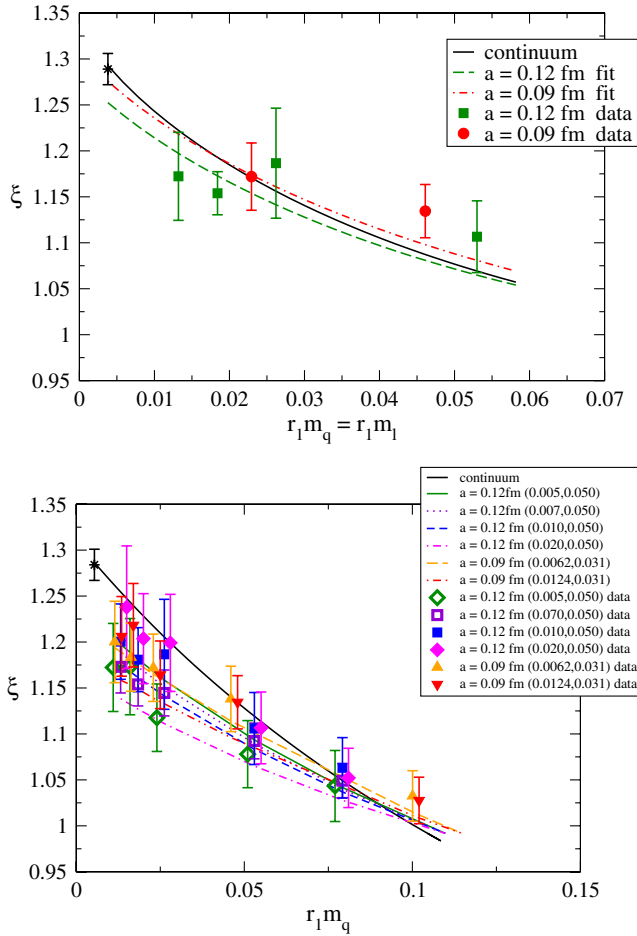


FIG. 5 (color online). Fits results using the NLO rHMS χ PT, first line in Eq. (5.6). The (black) star is the physical value of ξ in both panels. The top panel shows only the full QCD data, while the bottom one shows all the data included in the fits. The (green) squares and (red) circles and lines in the upper panel represent the 0.12 fm and 0.09 fm data and fit results, respectively. In the bottom panel, each color (symbol) labels a different ensemble.

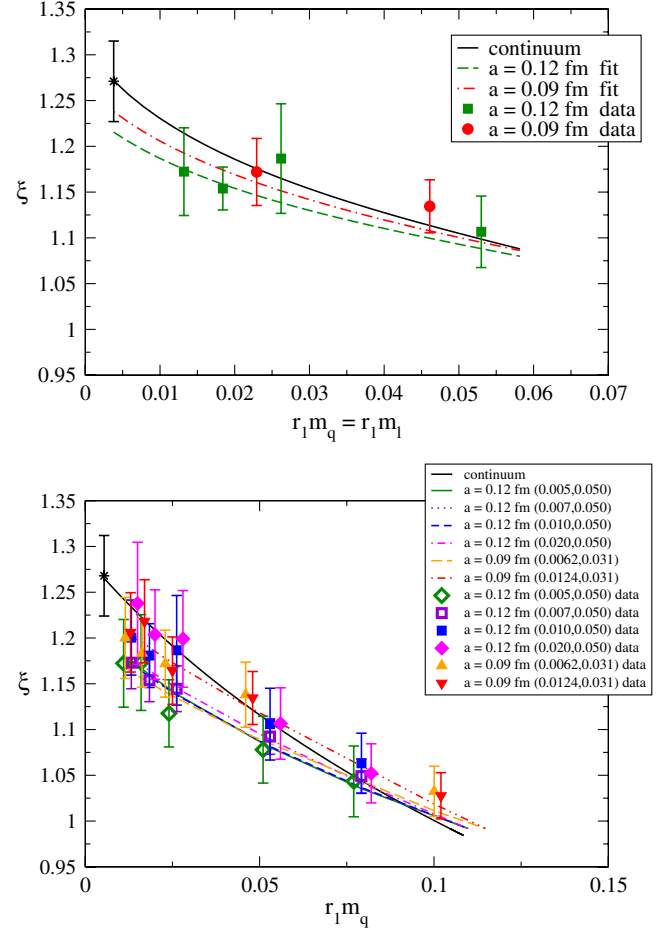


FIG. 6 (color online). Fits results using the NNLO rHMS χ PT in Eq. (5.6). The (black) star is the physical value of ξ in both panels. The top panel shows only the full QCD data, while the bottom one shows all the data included in the fits. The (green) squares and (red) circles and lines in the upper panel represent the 0.12 fm and 0.09 fm data and fit results, respectively. In the bottom panel, each color (symbol) labels a different ensemble.

$t_{\min}$, and this is repeated, reducing $t_{\min}$ until the $\chi^2/\text{d.o.f.}$ is no longer reasonable, ≈ 1.5 . Then an additional pair of states is added to the model function, and the process iterated. Once the time slice $t = 2$ can be included, that number of states is used in our central-value fits.²

For the three-point function, we fit using $N_{\text{states}} = N_{\text{regular}} + N_{\text{oscillating}} = 2 + 2 = 4$ and time slices $t_x, t_y \in [2, 10]$ for all ensembles. The two-point functions are fit for $t \in [2, 20]$ using $3 + 3$ states. The output of these fits successfully describe the oscillations in the correlation functions as can be seen in Fig. 3, which shows the typical behavior in one of the ensembles analyzed.

²Time slices $t = 0$ and $t = 1$ contain unconstrained contamination from higher-energy states. At $t = 0$ all states contribute because they have the same exponential weighting, and $t = 1$ is contaminated by higher-energy states because the degrees of freedom of staggered fermions spread over two time slices.

TABLE III. Number of states and time ranges used for each correlator in the fits for both the $a \approx 0.12$ fm and $a \approx 0.09$ fm ensembles. For the number of states, the first value indicates the number of regular states and the second one, the number of oscillating states. The labels between parentheses in the first column indicate the type of source/sink in that correlator.

Correlator	Number of states	Time range
$C_{\text{PS}}(\text{local/local})$	3 + 3	2–20
$C_{\text{PS}}(\text{local/1S})$	3 + 3	2–20
$C_{Q_q}(\text{local/1S})$	2 + 2	$(2 - 10) \times (2 - 10)$

In order to check that this number of states is sufficient, we add more states and examine the stability of the fits. Stability plots over numbers of states for the $a \approx 0.09$ fm ensembles, which illustrate the typical behavior of our fits, are shown in Fig. 4. The stability of central values and errors is very good for $N_{\text{states}} \geq 4$ in all cases.

V. CHIRAL PERTURBATION THEORY

The light sea- and valence-quark masses that are used in our lattice simulations have unphysically large values, with our lightest pion mass ≈ 240 MeV. To obtain information about the quark-mass dependence of the relevant matrix elements, which allows us to extrapolate our results to the physical masses, we perform our calculation at six sea $\times$ six valence quark masses, thus including numerous partially quenched data points. In addition, the leading-order taste violations, which arise at $O(a^2\alpha_s)$, are included in the theory and then removed when the extrapolation is performed using rooted heavy-meson staggered chiral perturbation theory (rHMS χ PT) [61,62,65]. The χ PT expression for $\langle \mathcal{O}_1^q \rangle$, as well as for the matrix elements of all the other operators in the $\Delta B = 2$ effective Hamiltonian, was first described in Ref. [85] for partially quenched Wilson-type quarks in the framework of continuum heavy-meson χ PT (HM χ PT). With staggered fermions, we also must include the effects of taste-violating interactions, using rHMS χ PT [65].

With the four-quark operators, a careful examination of the Fierz properties shows that there are additional operators with both wrong taste and *spin*, i.e., wrong (Γ_1, Γ_2) . As far as we know, this property of local heavy-staggered four-quark operators has not been discussed in the literature before. The needed rHMS χ PT expressions are derived in Ref. [86]. We became aware of these contributions after our analysis was nearly complete, so we have not included them in the chiral fit functions used here. We do, however, estimate the associated systematic error on ξ in our error budget (cf. Sec. VIC). Explicit expressions for the chiral fit functions used in this work are given in Appendix A.

The NLO rHMS χ PT in Eq. (A1) and subsequent equations in the appendix can be schematically written as

$$\begin{aligned} \langle \bar{B}_q | \mathcal{O}_1^q | B_q \rangle &= \frac{2}{3} M_{B_q}^2 f_{B_q}^2 B_q \\ &= M_{B_q} \alpha [1 + (\mathcal{W}_q + \mathcal{T}_q + \mathcal{Q}_q) + L_v m_q \\ &\quad + L_s (2m_l + m_h) + L_a a^2], \end{aligned} \quad (5.1)$$

where α , L_v , L_s , and L_a are low-energy constants (LECs) to be determined from fitting the data, the factor of M_{B_q} comes from the HQET normalization of states, and the masses m_q , m_l , and m_h are the light valence, light sea, and strange sea-quark masses, respectively. The light sea quarks are treated as degenerate, and the isospin average is used, i.e., $\hat{m} = (m_u + m_d)/2$. For staggered quarks, the taste-nonsinglet pseudoscalar meson masses are split

$$M_{ij,\rho}^2 = \mu(m_i + m_j) + a^2 \Delta_\rho, \quad (5.2)$$

where m_i and m_j are the quark masses and the sixteen meson masses are labeled by their taste representation, $\rho = P, A, T, V, I$. The parameters μ and the Δ_ρ 's are determined from lattice calculations for pions and kaons [87]. Their values are collected in Table IV.

The chiral logarithms, $\mathcal{W}_q$, $\mathcal{T}_q$, $\mathcal{Q}_q$, stem from wave function renormalization, tadpole, and sunset diagrams,

TABLE IV. Inputs for the priors of the free parameters and for the fixed parameters in the fits. The NLO low-energy constants L_v , L_s , and L_a are not constrained in the fits. The parameter s is given by the quantity $1/(8\pi^2(r_1 f_\pi)^2)$. We do not consider errors on the slope μr_1 or the taste splittings $r_1^2 a^2 \Delta_\rho$ because those have negligible effect on the final results. In the right-hand side table, the two last columns correspond to lattice spacings $a \approx 0.12$ fm and $a \approx 0.09$ fm. See the text for explanations of the choices of parameters.

Fit parameters (central value $\pm$ width)		
$a \approx 0.12$ fm	$(a \approx 0.09$ fm)	
β	1 ± 1	
$g_{B^* B \pi}$	0.51 ± 0.20	
$r_1^2 a^2 \delta'_V$	0.0 ± 0.07 $(0.0 \pm 0.07) \times 0.35$	
$r_1^2 a^2 \delta'_A$	-0.28 ± 0.06 $(-0.28 \pm 0.06) \times 0.35$	
L_v	Unconstrained	
L_s	Unconstrained	
L_a	Unconstrained	
Q_{1-4}	$0 \pm s^2$	
P_{1-3}	$0 \pm s^2$	
Input (fixed) parameters		
$a \approx 0.12$ fm	$a \approx 0.09$ fm	
$f_\pi r_1$	0.2106	
μr_1	6.234	6.382
$r_1^2 a^2 \Delta_P$	0	0
$r_1^2 a^2 \Delta_V$	0.439	0.152
$r_1^2 a^2 \Delta_T$	0.327	0.115
$r_1^2 a^2 \Delta_A$	0.205	0.0706
$r_1^2 a^2 \Delta_I$	0.537	0.206

respectively. The explicit expressions can be found in Appendix A.

In this work, we do not include the effects of the hyperfine splitting Δ^* or the light-flavor splittings δ_k defined in the Appendix. The wrong spin terms contribute to the tadpole and sunset diagrams [86].

When extrapolating to the physical point, we set the parameters Δ_ρ and $\delta'_{A,V}$ (which describe discretization effects) and the lattice spacing to zero, and set the sea quark masses to their physical values, $m_l \rightarrow (m_u + m_d)/2$, and $m_h \rightarrow m_s$. We then obtain $\langle \bar{B}_d^0 | \mathcal{O}_1^d | B_d^0 \rangle$ or $\langle \bar{B}_s^0 | \mathcal{O}_1^s | B_s^0 \rangle$ by setting $m_q = m_d$ or m_s . Thus, it is an extrapolation to the u - and d -quark masses and an interpolation to the s -quark mass.

An additional consideration is that $SU(3)$ NLO χ PT may not be valid for data with masses as large as the strange quark's. It would be desirable to include next-to-next-to-leading order (NNLO) contributions to test the validity of the NLO expression, but the effort needed to calculate the NNLO logs is prohibitive. It is reasonable instead to test the chiral expansion by including just NNLO analytic contributions. Wherever the quark masses or splittings are large enough for such analytic NNLO terms to be significant, the NNLO logarithms should be slowly varying and well approximated by the analytic terms. We follow this strategy and supplement the NLO rHMS χ PT expressions with NNLO analytic terms in our fits, with prior constraints estimated based on χ PT power counting as explained in the next section.

A. Parametrization of the chiral expression

Dimensionful quantities are extracted first in units of the lattice spacing and then converted to their physical values using the r_1 scale [88,89]. This absolute scale is defined as $r_1^2 F(r_1) = 1.0$, where $F(r_1)$ is the force between static quarks. In our chiral fits, all parameters are first converted to units of r_1 by multiplying by the relative scale r_1/a . The values for r_1/a on every MILC ensemble used in our calculation are listed in Table I. After the chiral-continuum extrapolation, we convert from r_1 units with a physical value of r_1 . We take the result obtained by combining the 2009 MILC determination of $r_1 f_\pi$ [90] and the PDG value of f_π [16]. Following Ref. [59], the error for r_1 is determined by averaging the MILC value with the HPQCD value in Ref. [91] and then by inflating the uncertainty to take conservatively into account the possible correlations coming from the use of the same configurations in both determinations. The final value we use is $r_1 = 0.3117(22)$ [59]. The error associated with r_1 has a very small effect on the dimensionless quantity ξ .

The dominant lattice artifacts to take into account in our rHMS χ PT expressions are expected to be taste-violating contributions of $O(a^2 \alpha_s^2)$, since the $O(a^2 \alpha_s)$ taste-violating effects are absent for asqtad quarks. We parametrize these effects in our fits by defining a quantity A_a^2 ,

which is the ratio of the size of taste violations on lattices with spacing a to those on the $a \approx 0.12$ fm lattices. Thus $A_{0.12 \text{ fm}}^2 = 1$ and

$$A_{0.09 \text{ fm}}^2 \equiv \frac{(\alpha_s^2 a^2)_{0.09 \text{ fm}}}{(\alpha_s^2 a^2)_{0.12 \text{ fm}}} \sim 0.35. \quad (5.3)$$

The NLO rHMS χ PT function in Eq. (5.1) can then be rewritten as

$$\begin{aligned} \beta_q &\equiv \sqrt{\frac{3}{2} \langle \bar{B}_q | \mathcal{O}_1^q | B_q \rangle} / M_{B_q} \\ &= f_{B_q} \sqrt{M_{B_q} B_{B_q}} \\ &= \beta^\chi \left[1 + \frac{1}{2} (\mathcal{Q}_q + \mathcal{W}_q + \mathcal{T}_q) + \frac{L_v}{2} M_{qq}^2 \right. \\ &\quad \left. + \frac{L_s}{2} (2M_{ll}^2 + M_{hh}^2) + \frac{L_a}{2} A_a^2 \right], \end{aligned} \quad (5.4)$$

where $\beta^\chi = \sqrt{\alpha}$. The masses M_{ij} are defined in Eq. (5.2), but here we disregard a^2 corrections in the masses since they can be absorbed by a redefinition of the low-energy constants at higher order in the chiral expansion. To the NLO expression above we add, inside the square brackets, the allowed NNLO analytic terms, which contribute with seven more unknown LECs

$$\begin{aligned} &Q_1 M_{qq}^4 + Q_2 (2M_{ll}^2 + M_{hh}^2)^2 + Q_3 M_{qq}^2 (2M_{ll}^2 + M_{hh}^2) \\ &+ Q_4 (2M_{ll}^4 + M_{hh}^4) + P_1 A_a^2 M_{qq}^2 + P_2 A_a^2 (2M_{ll}^2 + M_{hh}^2) \\ &+ P_3 A_a^4. \end{aligned} \quad (5.5)$$

In the above expressions, we have suppressed the factors of r_1 for simplicity. They can be deduced using dimensional considerations. In these expressions, which are the ones we use as fit functions, we write the analytic terms for convenience as functions of the pseudoscalar masses M_{ij} rather than the quark masses.

The ratio ξ can be extracted by first interpolating β_q to $m_q = m_s$ and extrapolating to $m_q = m_d$ separately according to expressions (5.4) and (5.5), and then forming the ratio β_s/β_d . Alternatively, one can consider the ratio of chiral expressions and expand up to NNLO to obtain

$$\begin{aligned} \xi' &= \frac{\beta_{q'}}{\beta_q} = \xi \frac{\sqrt{M_{B_{q'}}}}{\sqrt{M_{B_q}}} \\ &= 1 + \frac{1}{2} (\mathcal{Q}_{q'} + \mathcal{W}_{q'} + \mathcal{T}_{q'} - \mathcal{Q}_q - \mathcal{W}_q - \mathcal{T}_q) \\ &\quad + \frac{L_v}{2} (M_{q'q'}^2 - M_{qq}^2) + Q_1 (M_{q'q'}^4 - M_{qq}^4) \\ &\quad + Q_3 (M_{q'q'}^2 - M_{qq}^2) (2M_{ll}^2 + M_{hh}^2) \\ &\quad + P_1 (M_{q'q'}^2 - M_{qq}^2) A_a^2, \end{aligned} \quad (5.6)$$

with $m_{q'}$ fixed to the value closest to m_s . In Eq. (5.6) we disregard the NNLO terms coming from squaring the NLO terms in the denominator, since they are not necessary to obtain good fits and they are difficult to disentangle from those already included. We can then interpolate/extrapolate to $m_{q'} = m_s$ and $m_q = m_d$. We call these two strategies for the chiral and continuum extrapolation of ξ the indirect and direct methods, respectively. Many of the fit parameters cancel in the chiral expression for ξ' in Eq. (5.6), improving the reliability and stability of the fits. In addition, discretization errors of $O(\alpha_s \Lambda_{\text{QCD}} a, (\Lambda_{\text{QCD}} a)^2)$ from the heavy-quark action that are not included in the chiral perturbation theory, partially cancel in the ratio. We thus choose this method as our preferred fitting strategy.

B. Results from the chiral fits

In order to perform the chiral fits, we first create 200 bootstrap samples of β_q for each sea- and valence-quark mass combination from the two- and three-point correlator fits. The bootstrap data is then fit to the chiral expression using Bayesian techniques. The fits are simultaneously performed to all ensembles in Table I.

The input and fit parameters are set as in Table IV. We do not impose any constraint on the NLO low-energy constants. For the NNLO LECs we use prior widths based on a simple power counting argument. The NLO analytic terms should be of magnitude similar to the NLO logs, which are $\sim m_\pi^2/(8\pi^2 f_\pi^2) = s(r_1 m_\pi)^2$, (with $s \equiv 1/(8\pi^2(r_1 f_\pi)^2)$). Hence, the NNLO terms are $\sim (m_\pi^2/(8\pi^2 f_\pi^2))^2 = s^2(r_1 m_\pi)^4$. The taste-violating hairpin parameters, δ'_V and δ'_A , were also determined from lattice calculations for pions and kaons in Ref. [66]. We constrain the parameters δ'_V and δ'_A in our fits using the results of Ref. [66] as prior central values and widths. We also take the effective coupling of the $B^* B \pi$ interaction, $g_{B^* B \pi}$, as a fit parameter in our analysis. The prior central value and width we use for this parameter, shown in Table IV, covers the main ranges of determinations of $g_{B^* B \pi}$ [92–98], as discussed in Ref. [57]. A more recent, precise value of $g_{B^* B \pi}$, obtained with $N_f = 2 + 1$ domain-wall fermions and static b quarks [99], was not yet available when this stage of the analysis was carried out. Nevertheless, the result obtained by the authors in Ref. [99], $0.449 \pm 0.047 \pm 0.019$, falls well within the prior central value and width considered here. For the pion decay constant, we use the PDG value, $f_\pi = (130.41 \pm 0.20)$ MeV [16].

The fit results for ξ using different ansätze for the fitting function and the direct and indirect methods explained in Sec. VA are listed in Table V. The results and errors obtained using the direct and indirect methods agree very well, especially when NNLO terms are included. This constitutes a good check of how well our results are encompassing higher-order terms in the chiral expansion, which are different in these two methods.

TABLE V. Results from the rHMS χ PT fits. Errors are only statistical and obtained from 200 bootstrap samples. For a full discussion of systematic errors, see Sec. VI.

Ansatz	$\chi^2/\text{d.o.f.}$	ξ Direct	$\chi^2/\text{d.o.f.}$	ξ Indirect
NNLO	0.45	$1.268^{+0.035}_{-0.044}$	0.23	$1.255^{+0.034}_{-0.041}$
NLO	0.78	$1.284^{+0.018}_{-0.016}$	0.49	$1.262^{+0.008}_{-0.012}$

In Figs. 5 and 6, we show the NLO and NNLO fit results for ξ from the direct method as a function of the light valence mass in r_1 units, $r_1 m_q$. The top panels in both figures show only the full QCD points, $m_q = m_l$, while the bottom panels show all (partially quenched) data included in the fits (see Table I). The fit curve is the same in both panels of each figure. The black lines show the results of the fit in the continuum limit, after the dominant lattice artifacts are removed using rHMS χ PT, and after interpolating the physical sea and valence strange-quark masses to the physical value, as a function of the valence light-quark mass. The black point is our result for ξ at the physical masses, and includes statistical errors.

From the spread of data in the bottom panels of both figures (same data), one can see that the light sea-quark mass dependence is mild; all different sea-quark masses (squares or triangles at a particular axis value) agree within one statistical σ . The discretization errors are also small, as can be seen in both the data and the extrapolation lines in the upper panels.

We obtain fits that match the data well and have good $\chi^2/\text{d.o.f.}$ with only the inclusion of NLO terms, as shown in Fig. 5. When we add the NNLO terms, the central values for ξ are also within one statistical σ , although errors are significantly larger. This is to be expected, since the NNLO LECs are poorly known. Related to this is the fact that the $\chi^2/\text{d.o.f.}$ for the NLO fits are larger than for the NNLO fits. At NNLO, we are including extra degrees of freedom with large prior widths that are poorly determined by the fit, so, in practice, we are dividing the same χ^2 by a larger number of degrees of freedom. In fact, the NNLO fits seem to give a slightly better description of the data, as can be seen in the full QCD plots. The chiral extrapolation for ξ is also milder in the NNLO case. Based on these arguments and, as mentioned above, the fact that direct and indirect fits agree better at NNLO, we choose the direct NNLO fit for our central value and statistical error. The systematic error associated with our choice of fit function is discussed in Sec. VID.

VI. ERROR ANALYSIS

In this section, we discuss all sources of systematic uncertainty affecting our calculation of ξ . The systematic errors have to be added to the statistical uncertainty listed in Table V, which also encompasses our imperfect knowledge about chiral parameters such as $g_{B^* B \pi}$ and $\delta'_{V,A}$.

A. Heavy-quark mass uncertainty

The mixing parameters depend on the b quark mass used in our simulations through the hopping parameter κ_b , which is tuned so that the kinetic meson mass, M_2 , agrees with the experimental result. The dispersion relation for a heavy particle can be written for low-momentum as

$$E(\mathbf{p}) = M_1 + \frac{\mathbf{p}^2}{2M_2} - \frac{a^3 W_4}{6} \sum_j p_j^4 - \frac{(\mathbf{p}^2)^2}{8M_4^3} + O(\mathbf{p}^6), \quad (6.1)$$

where κ_b enters into the definitions of M_1 and M_2 [40]. W_4 and the deviation of M_4 from M_2 capture lattice artifacts. We calculated two-point functions for the pseudoscalar and vector mesons at several momenta and extract the energy, $E(\mathbf{p})$, for each particle at each momentum. A fit to the dispersion relation then determines M_2 and the spin average of the results is taken. The κ_b value is then adjusted until M_2 agrees with the spin-averaged B_s meson mass.

In this work, we use the values for κ_b on the $a \approx 0.12$ fm and $a \approx 0.09$ fm ensembles tuned this way in Ref. [55]. The error in the determination translates into a systematic error in the mixing matrix elements. However, in the ratio ξ the effect of the uncertainty is minimal, since the corrections go in the same direction in both denominator and numerator, and, thus, largely cancel. In addition, most of the remaining dependence is encoded in the decay constants rather than in the bag parameters, which are very insensitive to the exact values of the quark masses. In Ref. [59], we studied the decay constants with the same choice of actions, parameters, and configurations as here. We expect systematic errors to be very similar in both analyses. We therefore, adopt the error due to the uncertainty in the b quark mass obtained in Ref. [59] for the ratio of decay constants f_{B_s}/f_{B_d} , namely, 0.4%, as a good estimate of this systematic error for ξ .

B. Higher-order effects in the perturbative matching

The most straightforward and conservative way to estimate the effects of the missing higher order terms in the perturbative matching is to assume two-loop coefficients of order 1 and to multiply the central value by $\alpha_s^2 = \alpha_V^2(2/a)$. This estimate gives an error $\sim 5\%$ for $f_B\sqrt{B_B}$ on the $a \approx 0.12$ fm lattices and $\sim 3.6\%$ on the $a \approx 0.09$ fm lattices, becoming the main source of uncertainty for this quantity [37]. If there was no mixing between $\langle \mathcal{O}_1 \rangle$ and $\langle \mathcal{O}_2 \rangle$ under renormalization, there would be an exact cancellation of the renormalization coefficients for the ratio $\xi = (f_{B_s}\sqrt{B_{B_s}})/(f_{B_d}\sqrt{B_{B_d}})$, as long as the valence light-quarks are taken to be massless in the renormalization calculation. The mixing under renormalization prevents this exact cancellation from happening, but the renormalization corrections in the ratio are still largely suppressed, by a factor of $\langle \mathcal{O}_2^s \rangle / \langle \mathcal{O}_1^s \rangle - \langle \mathcal{O}_2^d \rangle / \langle \mathcal{O}_1^d \rangle$, with respect to those for a single matrix element. We estimate this suppression factor via the

ratio $(m_s - m_d)/\Lambda_{\text{QCD}}$ and multiply the perturbative error for $f_B\sqrt{B_B}$ given above by it. As a result, the perturbative matching uncertainty for ξ from this estimate is 0.2–0.5% (for $\Lambda_{\text{QCD}} = 700$ MeV).

The ratio ξ changes by 0.2% when the one-loop renormalization is omitted entirely, supporting our power counting argument. Another way of estimating $O(\alpha_s^2)$ effects is by varying the scale q^* at which α_V is evaluated. If we change q^* from our central value of $2/a$ to $1/a$ and $3/a$ we find that the extrapolated ξ changes between 0.2 and 0.4%.

Since the initial estimate yields the largest uncertainty, 0.5%, we take this as the error associated with the missing higher order terms in the perturbative renormalization. Hence, this source of uncertainty is subdominant in our determination of ξ .

C. Mixing with wrong spin four-fermion operators

As mentioned in Sec. V, there are contributions at NLO in rHMS χ PT originating from the mixing of $\langle \mathcal{O}_1 \rangle$ with the matrix elements of four-fermion operators of different spin and taste. We have omitted these contributions from our chiral fits, because we discovered these terms after this stage of the analysis was complete. From Figs. 5 and 6, one can see that the effect of the wrong spin mixing is unlikely to be very large, perhaps being mostly absorbed into the LECs.

We cannot include the effects of the wrong spin contributions, because they require the matrix elements of $\mathcal{O}_3$, which we have not computed here. Fortunately, however, we have started a more comprehensive analysis of B - $\bar{B}$ mixing on a larger set of higher-statistics ensembles, including $\mathcal{O}_3$. We have added the wrong spin operators to that analysis and find that their inclusion tends to increase the slope of the continuum extrapolated chiral fit function for $\langle \mathcal{O}_1 \rangle$ and, hence, ξ . For example, taking priors and widths similar to those in Table IV, we find a 2% increase in ξ , while for other reasonable choices of the priors the variation is not larger than 3.2%. We add a 3.2% systematic error to account for the missing terms in our chiral extrapolation functions.

D. Chiral-extrapolation systematics and light-quark discretization

The errors due to the choice of fit ansatz and light-quark discretization effects cannot be disentangled, because every fit ansatz necessarily treats the discretization errors differently. So any estimate of the systematic uncertainty associated with the choice of ansatz also accounts for the light-quark discretization errors left over after removing the dominant ones using rHMS χ PT.

In Fig. 7, we show the distribution of values for ξ obtained with the NNLO direct fit for the 200 bootstrap samples analyzed. We check that 200 bootstrap samples is enough to obtain a (nearly) Gaussian distribution, as can be seen in the panel. With the goal of testing our choice of

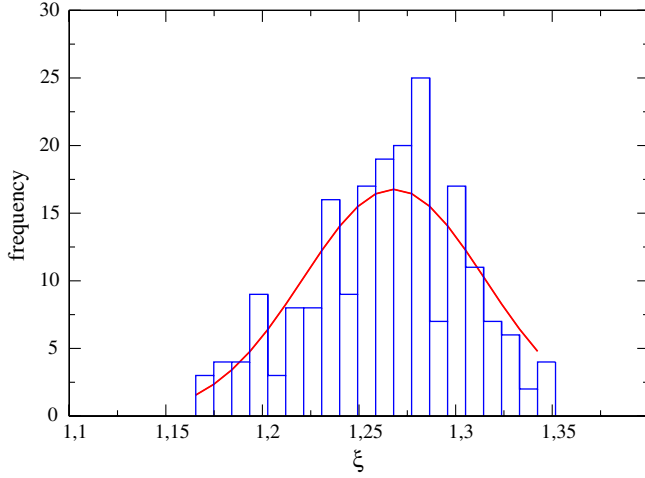


FIG. 7 (color online). Histogram of the distribution of values of ξ obtained from the 200 bootstrap samples. The curve is a Gaussian distribution corresponding to $\xi = 1.268 \pm 0.047$ (the NNLO result with augmented errors as explained in the text).

functional form and the error associated with the truncation of the chiral series, we perform fits with only two of the three NNLO terms, omitting each one in turn. All fits give good values of $\chi^2/\text{d.o.f.}$ and p value. The values of ξ obtained are scattered around the distribution in Fig. 7 but always within 1.5 statistical σ of the central value. This consistency, together with the fact that the NNLO LECs are not well determined by the fit, indicates that the statistical error already accounts for the possibility of having one of the unknown constants equal or close to zero. If we inflate and symmetrize our statistical errors to ± 0.047 , we cover the spread of results from the different fitting functions tried (including the NLO one). We take this value as our estimate of both statistical and chiral systematic uncertainties.

An alternative way of estimating the uncertainty in the truncation of the chiral series and the fitting function would be taking the difference between the NLO and the NNLO fits results. If we add this difference with the statistical errors in Table V in quadrature, the uncertainty would be slightly smaller than the ± 0.047 we are taking as our estimate of these two sources of error.

In the rest of this section, we list the errors associated with the uncertainty of several input parameters used in the continuum and chiral fits, that typically can be estimated by varying the inputs and redoing the fits.

1. Light-quark mass uncertainty

The physical values of the light-quark masses used for the extrapolations and interpolations for ξ are determined by the MILC collaboration [87,100]. They are obtained by making the charged pions and kaons take on their physical values after removal of electromagnetic effects and are listed in Table VI.

TABLE VI. Input for the physical light-quark masses used in the chiral extrapolations. These values were determined by the MILC collaboration [87,100]. Physical values are found from chiral fits that have been extrapolated to the continuum, but masses are still in units of the $a \approx 0.09$ fm lattice spacing.

Quantity	Physical
$am_s \times 10^2$	2.72 (8)
$a \frac{(m_u+m_d)}{2} \times 10^3$	0.997 (35)
$am_d \times 10^3$	1.40(6)

The error on ξ due to the light-quark mass uncertainties is obtained by individually varying each quark mass within this uncertainty and repeating the preferred chiral fit and extrapolation. The central values arrived at using each mass variation are compared to the results of the fit which used the central values for the masses, and their differences are added in quadrature. This gives a total systematic error due to the light-quark mass uncertainties of 0.5% for ξ .

2. Uncertainty in the scale r_1

The value of r_1 used in this analysis to convert from lattice to physical units, as described in Sec. VA, is $r_1 = 0.3117(22)$ fm. The results discussed in previous sections are obtained by fixing r_1 to its central value. In order to estimate the uncertainty due to the error in r_1 we change r_1 by ± 0.0022 fm and all parameters that depend on the physical r_1 are appropriately adjusted. The uncertainty in scale gives a systematic error of 0.2%, which is very small due to the fact that ξ is a dimensionless quantity and the scale only enters in the normalization to lattice units of the chiral corrections $(1/(f_\pi r_1)^2)$ and indirectly via the tuning of the quark masses.

E. Heavy-quark discretization effects

The discretization errors associated with our choice of heavy-quark action to simulate the bottom quarks can be described in terms of the difference in the lattice and continuum Wilson coefficients of higher dimension operators in the HQET expansion. Those come from two sources: the mismatch between continuum and lattice in the Lagrangian and the mismatch in the four-fermion operators whose matrix elements yield $f_B \sqrt{B_B}$ and, thus, ξ . For a particular operator Q_i the error can be written in terms of the usual power counting magnitudes times functions that reflect the particular $m_0 a$ dependence of the action [56,101]

$$\text{error}_i = z_i f_i(m_0 a) (a \Lambda_{\text{QCD}})^{s_i}, \quad (6.2)$$

where $s_i = \dim Q_i - 4$ for Lagrangian operators Q_i of dimension 4 and 5, and $s_i = \dim Q_i - 6$ for four-fermion operators Q_i of dimension 7 and 8, and the z_i are constants. The functions $f_i(m_0 a)$ can be deduced from Refs. [40,102] and were discussed in detail in Ref. [56] for the form

factors parametrizing $B \rightarrow \pi l \nu$ decays and in Ref. [59] for heavy-light decay constants. A detailed study of these corrections for the matrix elements of all the operators contributing to neutral B mixing in the SM and beyond will be presented elsewhere [77]. Here we only summarize the sources of the different corrections for $\langle \mathcal{O}_1 \rangle$ and ξ . The explicit form of the different functions $f_i(m_0 a)$ can be found in Appendix B.

From the Lagrangian, there are $O(a^2)$ errors and $O(\alpha_s a)$ errors which are identical to those in Eqs. (A12) and (A19) in Ref. [59]. They are proportional to the functions $f_E(m_0 a)$ in Eq. (B1) and $f_B(m_0 a)$ in Eq. (B2) of Appendix B, respectively.

From the four-fermion operators, we have $O(a^2)$ errors coming from higher order corrections to the rotation relation in Eq. (2.29). They are generated by the mismatch between lattice and continuum coefficients of the operators $\bar{q} \Gamma D^2 b$, $\bar{q} \Gamma i \cdot B b$ and $\bar{q} \Gamma \alpha \cdot E b$ in the same way as in Eqs. (A13) and (A14) of Ref. [59], but with an extra overall factor of two due to the fact that we have two heavy fields in our leading-order operator, not one. These corrections are proportional to the functions $f_X(m_0 a)$ and $f_Y(m_0 a)$ in Eq. (B3) of Appendix B, respectively.

The last contribution, and the least straightforward, comes from the $O(\alpha_s a)$ corrections to the four-fermion operators. In principle, to subleading order, there are a basis of twelve new local operators in the effective Hamiltonian. However, using symmetry constraints, Fierz transformations, and rewriting some combinations as total derivatives, only five independent operators remain [37,103]. Because we separate the temporal and spatial parts of the operators through this analysis, the total temporal and spatial components of those five operators should be compared with the temporal and spatial parts of the leading operators. As explained in Ref. [77], this produces a difference of $3f_3(m_0 a)$, where f_3 is given in Eq. (B4).

In Table VII, we list all the contributions together with the functions f_i , and the proportionality constant z_i in Eq. (6.2). We also list the numerical values of the different contributions to the heavy-quark discretization error in percentage for $f_B \sqrt{B_B}$. In order to get the numerical results, we use $\Lambda_{\text{QCD}} = 700$ MeV and $\alpha_s = \alpha_V(2/a)$ listed in Table II. The final heavy-quark discretization error for

TABLE VII. Heavy-quark discretization errors given in percentages.

Contribution	f_i	z_i	Error $f_B \sqrt{B_B}$ (%) (coarse,fine)	Error ξ (%) (coarse,fine)
$\mathcal{O}(a^2)$ Lagrangian	f_E	2	(0.28,0.16)	
$\mathcal{O}(a_s a)$ Lagrangian	f_B	2	(0.96,0.58)	
$\mathcal{O}(a^2)$ Operator	f_X	4	(1.29,0.74)	
	f_Y	2	(0.23,0.18)	
$\mathcal{O}(a_s a)$ Operator	f_3	3	(1.32,0.75)	
Total error			(2.1,1.3)	(0.2,0.1)

$f_B \sqrt{B_B}$ is 1.3% for the $a \approx 0.09$ fm ensembles and 2.1% for the 0.12 fm ones.

These errors largely cancel in ξ . The effect of the cancellation on the error can be estimated by multiplying the errors in $f_B \sqrt{B_B}$ by a factor of $(m_s - m_d)/\Lambda_{\text{QCD}}$ which gives a final heavy-quark discretization error for ξ of 0.2% for the coarse lattice and 0.1% for the fine lattice. This agrees well with the estimate of this type of error for the ratio f_{B_s}/f_B [59], $\sim 0.3\%$, using a very similar set of data and statistics. The strategy followed in Ref. [59] differs from the one described here. In that paper, terms of the form in Eq. (6.2) were directly added to the chiral and continuum extrapolation fitting functions with a coefficient of order one to be determined by the fit. Ultimately, we would like to employ that strategy also for $B^0 - \bar{B}^0$ mixing studies. For this work, however, we simply take the larger estimate from the ratio f_{B_s}/f_B as our estimate of the uncertainty in ξ due to heavy-quark discretization errors.

F. Finite volume corrections

In order to evaluate the finite volume corrections in our calculation, we follow the prescription in Refs. [65,104]. The MILC lattices are large enough in the time direction that it can be treated as infinite to a very good approximation, so we are interested in corrections due to finite spatial volume only. They are estimated by replacing infinite-volume integrals in the chiral expression with finite sums over the spatial momentum.

Including finite volume corrections in the chiral expressions and redoing the fits reveals negligible errors, $< 0.1\%$.

G. Tuning of the tadpole parameter u_0

The tadpole improvement factor u_0 is a parameter of the gauge and asqtad staggered (sea) quark action and is determined from the fourth root of the average plaquette. The tadpole improvement factor also enters into the valence light and heavy quark actions. On the $a \approx 0.09$ fm ensembles, the valence quarks are generated with the same values of u_0 as the sea. However, on the $a \approx 0.12$ fm ensembles, the valence quark actions use values of u_0 obtained from the average link in Landau gauge instead. The differences between the values of u_0 obtained with the two methods is around 3–4%.

The effect on f_{B_s}/f_B of the mismatch between u_0 values in the valence and the sea sectors of the $a \approx 0.12$ fm ensembles was estimated to be $< 0.1\%$ in Ref [59]. Since this is much smaller than the errors due to statistics, chiral fits, and continuum and chiral extrapolation, we take this estimate as our error on ξ .

VII. DISCUSSION OF RESULTS AND FUTURE IMPROVEMENTS

The error budget for the $SU(3)$ -breaking mixing parameter ξ described in the previous sections is summarized

TABLE VIII. Complete error budget and total error for the B^0 mixing parameter ξ . All errors are given in percentages.

Source of uncertainty	Error (%)
Statistics $\oplus$ light-quark disc. $\oplus$ chiral extrapolation	3.7
Mixing with wrong-spin operators	3.2
Heavy-quark discretization	0.3
Scale uncertainty (r_1)	0.2
Light-quark masses	0.5
One-loop matching	0.5
Tuning κ_b	0.4
Finite volume	0.1
Mistuned coarse u_0	0.1
Total error	5.0

in Table VIII. For the first error in the table we prefer not to attempt to disentangle the statistical, light-quark discretization, and chiral extrapolation errors since, as explained in Sec. VID, the lack of knowledge about the LECs at NNLO makes a reliable separation impossible. Our final result is

$$\xi = 1.268 \pm 0.063. \quad (7.1)$$

The total uncertainty is dominated by the combined statistical, light-quark discretization, and chiral extrapolation error, and the uncertainty associated with the wrong spin operators in the chiral-continuum extrapolation.

Combining our result in Eq. (7.1) with the averages of the experimentally measured values of the mass differences $\Delta M_d = (0.507 \pm 0.004) \text{ ps}^{-1}$ [16] and $\Delta M_s = (17.69 \pm 0.08) \text{ ps}^{-1}$ [105], and the meson masses $M_{B_s^0} = (5366.0 \pm 0.9) \text{ MeV}$ and $M_{B_d^0} = (5279.5 \pm 0.5) \text{ MeV}$ [16], we quote a value for the ratio of the CKM matrix elements

$$\left| \frac{V_{td}}{V_{ts}} \right| = 0.216 \pm 0.011, \quad (7.2)$$

assuming no new physics in $B_{(s)}^0$ - $\bar{B}_{(s)}^0$ mixing. The error includes the uncertainties in the B -meson masses and mass differences but it is strongly dominated by the error in ξ .

We can also take our result for ξ and combine it with the value of the decay constant ratio $f_{B_s}/f_{B_d} = 1.229 \pm 0.026$ calculated by our collaboration [59] to determine the ratio of bag parameters

$$\frac{B_{B_s}}{B_{B_d}} = \xi^2 \left(\frac{f_{B_d}}{f_{B_s}} \right)^2 = 1.06 \pm 0.11. \quad (7.3)$$

The two results for ξ and f_{B_s}/f_{B_d} are correlated, but the statistical analyses were done independently so we cannot include the correlations in calculating the uncertainty in the ratio of bag parameters. Therefore, the error shown in the result of Eq. (7.3) is overestimated. However, as part of the future work, we plan to perform a common analysis of matrix elements and decay constants, from which we will

be able to account for correlations in extracting the value of the bag parameters and thus greatly reduce the error in Eq. (7.3). We will do the same for the individual bag parameters corresponding to all the operators in the basis in Eq. (1.3).

Our result for ξ in Eq. (7.1) is in good agreement with the HPQCD value obtained in Ref. [32], $\xi = 1.258(33)$. Note, however, that HPQCD did not estimate the effects of the wrong spin operators that appear in the complete NLO chiral expression, so the full error in their result may be somewhat bigger than what was quoted. The agreement of these two determinations of ξ provides an excellent check of the methodology and systematic error study in both analyses. In addition, it helps to increase the confidence in the robustness of lattice results for a parameter of great importance in phenomenological studies. In this article, we have established and tested the methodology to apply to broader studies of B^0 mixing with the same lattice formulations for light and bottom quarks as used here.

Statistical errors could be reduced significantly by expanding the analysis to include the full set of available configurations (approximately 2000) at each of the $a \approx 0.12 \text{ fm}$ and $a \approx 0.09 \text{ fm}$ ensembles. The current runs of our collaboration on the extended ensembles are also implementing sources located at a random spatial and time location to reduce further the statistical errors. We expect a reduction of the statistical errors by about a factor of two.

The other dominant error of our calculation, the omission in the rHMS χ PT analysis of terms generated by wrong spin operators, will be eliminated when a complete analysis is done with the full rHMS χ PT expressions [86]. A result for ξ that properly includes the wrong spin terms requires the calculation of the continuum matrix elements not only of the operator $\mathcal{O}_1$ as we have done in this work, but also of $\mathcal{O}_2$ and $\mathcal{O}_3$, and simultaneous chiral and continuum extrapolations of all three matrix elements.

The discretization errors, related to both heavy and light quarks, will be reduced in a straightforward way by simulations at smaller lattice spacing, i.e., on the $a \approx 0.06 \text{ fm}$ and $a \approx 0.045 \text{ fm}$ MILC lattices. The reduction of both statistical and discretization errors will also yield cleaner and more accurate continuum and chiral extrapolations. Including data at smaller lattice spacings will also reduce the uncertainty associated with the perturbative matching from the reduction of $\alpha_s = \alpha_V(2/a)$. Although not relevant for the reduction of the total error in ξ , this will be important in the determination of the matrix elements $\langle \mathcal{O}_i \rangle$ themselves.

Similarly, although the uncertainty associated with heavy-quark discretization effects is a subdominant source of error in the determination of ξ , it is one of the main errors in the determination of $\langle \mathcal{O}_i \rangle$ [37]. In order to have a more reliable, data-driven estimation of these effects, in our on-going analyses we plan to employ the strategy used in Ref. [59], in which terms like the ones in Eq. (6.2) are

included in the chiral-continuum extrapolation fitting form with free parameters to be determined from the fit.

Our new analysis, which incorporates the improvements mentioned above, includes the study of the matrix elements of all five operators that contribute to $H_{\text{eff}}^{\Delta B=2}$ [29]. This will allow not only the precise SM determination of $\Delta M_{s,d}$, $\Delta \Gamma_{s,d}$, and ξ , but will also provide the nonperturbative inputs needed to put constraints on BSM models using experimental data on B^0 mixing and related observables.

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APPENDIX A: STAGGERED CHIRAL PERTURBATION THEORY FOR B^0 - $\bar{B}^0$ MIXING

In this appendix we describe the functional form we use in the chiral and continuum extrapolation of the matrix elements $\langle \bar{B}_q^0 | \mathcal{O}_1^q | B_q^0 \rangle$. Further discussion, as well as complete NLO rHMS χ PT expressions for $\langle \bar{B}_q^0 | \mathcal{O}_1^q | B_q^0 \rangle$ with $i = 1, \dots, 5$ and the corresponding bag parameters can be found in Ref. [86].

At NLO in rHMS χ PT and at first order in the heavy-quark expansion we use

$$\langle \bar{B}_q^0 | \mathcal{O}_1^q | B_q^0 \rangle = \alpha \left(1 + \frac{\mathcal{W}_{q\bar{b}} + \mathcal{W}_{b\bar{q}}}{2} + \mathcal{T}_q + \mathcal{Q}_q \right) + L_v m_q + L_s (2m_l + m_h) + L_a a^2. \quad (\text{A1})$$

α , L_v , L_s , and L_a are constants to be determined from the fits to lattice data. The quantities in script for the partially quenched $2 + 1$ ($m_u = m_d \neq m_s$) case are

$$\begin{aligned} \mathcal{W}_{q\bar{b}} &= \mathcal{W}_{b\bar{q}} \\ &= \frac{ig_{B^*B\pi}^2}{f_\pi^2} \left[\frac{1}{16} \sum_{S,\rho} N_\rho \mathcal{H}_{Sq,\rho}^{\Delta^* + \delta_{Sq}} + \frac{1}{3} \left[R_{X_l}^{[2,2]}(\{M_{X_l}^{(5)}\}; \{\mu_l\}) \frac{\partial \mathcal{H}_{X,l}^{\Delta^*}}{\partial m_{X_l}^2} - \sum_{j \in \{M_l^{(5)}\}} D_{j,X_l}^{[2,2]}(\{M_{X_l}^{(5)}\}; \{\mu_l\}) \mathcal{H}_{j,l}^{\Delta^*} \right] \right. \\ &\quad \left. + a^2 \delta'_V \left[R_{X_v}^{[3,2]}(\{M_{X_v}^{(7)}\}; \{\mu_v\}) \frac{\partial \mathcal{H}_{X,v}^{\Delta^*}}{\partial m_{X_v}^2} - \sum_{j \in \{M_v^{(7)}\}} D_{j,X_v}^{[3,2]}(\{M_{X_v}^{(7)}\}; \{\mu_v\}) \mathcal{H}_{j,v}^{\Delta^*} \right] + (V \rightarrow A) \right], \end{aligned} \quad (\text{A2})$$

$$\begin{aligned} \mathcal{T}_q &= \frac{-i}{f_\pi^2} \left[\frac{1}{16} \sum_{S,\rho} N_\rho I_{qS,\rho} + \frac{1}{16} \sum_{\rho} N_\rho I_{X,\rho} + \frac{2}{3} \left[R_{X_l}^{[2,2]}(\{M_{X_l}^{(5)}\}; \{\mu_l\}) \left(\frac{\partial I_{X_l}}{\partial m_{X_l}^2} \right) - \sum_{j \in \{M_l^{(5)}\}} D_{j,X_l}^{[2,2]}(\{M_{X_l}^{(5)}\}; \{\mu_l\}) I_j \right] \right. \\ &\quad \left. + a^2 \delta'_V \left[R_{X_v}^{[3,2]}(\{M_{X_v}^{(7)}\}; \{\mu_v\}) \left(\frac{\partial I_{X_v}}{\partial m_{X_v}^2} \right) - \sum_{j \in \{M_v^{(7)}\}} D_{j,X_v}^{[3,2]}(\{M_{X_v}^{(7)}\}; \{\mu_v\}) I_j \right] + (V \rightarrow A) \right], \end{aligned} \quad (\text{A3})$$

$$\mathcal{Q}_q = \frac{-ig_{B^*B\pi}^2}{f_\pi^2} \left[\frac{1}{16} \sum_{\rho} N_\rho \mathcal{H}_{X,\rho}^{\Delta^*} + \frac{1}{3} \left[R_{X_l}^{[2,2]}(\{M_{X_l}^{(5)}\}; \{\mu_l\}) \left(\frac{\partial \mathcal{H}_{X,l}^{\Delta^*}}{\partial m_{X_l}^2} \right) - \sum_{j \in \{M_l^{(5)}\}} D_{j,X_l}^{[2,2]}(\{M_{X_l}^{(5)}\}; \{\mu_l\}) \mathcal{H}_j^{\Delta^*} \right] \right]. \quad (\text{A4})$$

In the equations above, the index ρ runs over the taste representation (P, A, T, V, I) with degeneracies N_ρ ($N_\rho = 1, 4, 6, 4, 1$, respectively), and S runs over the sea flavors u, d, s . The meson X is made of two light valence quarks q , and m_X is its mass. The functions $\mathcal{H}$ and I are the integrals defined in Appendix A of Ref. [85]. The subscripts on those functions label the flavor and taste of the meson masses at which they are evaluated.

The superscript in $\mathcal{H}$ is the second argument for that function as defined in Ref. [85]. In addition to the hyperfine splitting $\Delta^* = M_{B^*} - M_B$, it includes a light flavor splitting δ_{Sq} whenever the light flavor of the vector meson in the loop is different from the external flavor.

The splitting is $\delta_{Sq} \equiv M_{B^0_S} - M_{B^0_q} = 2\lambda_1 \mu (m_S - m_q)$, where λ_1 and μ are low-energy constants. The constant λ_1 comes from heavy quark effective theory, and μ is defined in Eq. (5.2).

The residue functions $R_j^{[n,k]}$ and $D_{j,l}^{[n,k]}$ in the expressions above are defined by Ref. [63]

$$R_j^{[n,k]}(\{m\}, \{\mu\}) \equiv \frac{\prod_{a=1}^k (\mu_a^2 - m_j^2)}{\prod_{i \neq j} (m_i^2 - m_j^2)}, \quad (A5)$$

$$D_{j,l}^{[n,k]}(\{m\}, \{\mu\}) \equiv -\frac{d}{dm_j^2} R_j^{[n,k]}(\{m\}, \{\mu\}).$$

The mass combinations appearing as arguments of these functions in the 2 + 1 partially quenched theory are

$$\begin{aligned} \{M_X^{(S)}\} &= \{m_\eta, m_X\}, \\ \{M_X^{(7)}\} &= \{m_\eta, m_{\eta'}, m_X\}, \\ \{\mu\} &= \{m_L, m_H\}, \end{aligned} \quad (A6)$$

where m_L is the meson mass made from $l\bar{l}$ sea quarks, and m_H is the meson mass made from $h\bar{h}$ sea quarks. The tastes of these mesons are indicated explicitly in the equations above.

Since we are not including the effects of the hyperfine splitting Δ^* or the light flavor splittings δ_k in this work, the functions $\mathcal{H}$ and I appearing in the wave function, tadpole, and sunset contributions simplify to

$$i\mathcal{H}_{k,\Xi}^0 = -3iI_{k,\Xi} = -\frac{3}{16\pi^2} M_{k,\Xi}^2 \ln\left(\frac{M_{k,\Xi}^2}{\Lambda_X^2}\right). \quad (A7)$$

APPENDIX B: FUNCTIONS PARAMETRIZING HEAVY-QUARK DISCRETIZATION ERRORS

In this appendix we collect the functions f_i needed in Eq. (6.2) to estimate the heavy-quark discretization errors affecting our calculation. For details on the origin of these functions and the effects of higher-dimension operators in the Lagrangian, see Ref. [102]. For further details on the application to the estimation of heavy-quark discretization errors in B^0 - $\bar{B}^0$ mixing, see Ref. [77].

(i) $O(a^2)$ errors from the Lagrangian:

$$f_E(m_0a) = \frac{1}{2} \left[\frac{(1 + m_0a) - 1}{m_0a(2 + m_0a)(1 + m_0a)} - \frac{1}{4(1 + m_0a)^2} \right]. \quad (B1)$$

(ii) $O(\alpha_s a)$ errors from the Lagrangian:

$$f_B(m_0a) = \frac{\alpha_s}{2(1 + m_0a)}. \quad (B2)$$

(iii) $O(a^2)$ errors from the four-fermion operator:

$$f_X(m_0a) = \frac{1}{2} \left[\frac{1}{2(1 + m_0a)} - \left(\frac{m_0a}{2(2 + m_0a)(1 + m_0a)} \right)^2 \right] \quad (B3)$$

$$f_Y(m_0a) = \frac{2 + 4m_0a + (m_0a)^2}{4(1 + m_0a)^2(2 + m_0a)^2}.$$

(iv) $O(\alpha_s a)$ errors from the four-fermion operator:

$$f_3(m_0a) = \frac{\alpha_s}{2(2 + m_0a)}. \quad (B4)$$

APPENDIX C: PRIOR CENTRAL VALUES AND WIDTHS FOR THE CORRELATOR FITS

In Table IX we collect the prior central values and widths used in the correlator fits described in Sec. IV. The amplitude parameters are defined in Eqs. (2.21) and (2.22), and the energy differences are defined as $\Delta E_{i+1,i} \equiv a(E_{i+1} - E_i)$.

TABLE IX. The priors with index 0 refer to the ground state. Superscripts d and $1S$ refer to the local and $1S$ smeared sources, respectively. Higher-energy state priors have indices i and j . The prime in E'_i refers to an opposite parity (oscillating) state.

	Prior central value	Prior width
Z_0^{1S}	2.2	0.5
Z_i^{1S}	0.01	0.5
Z_0^d	0.45	0.45
Z_i^d	0.01	1
O_{00}	0.01	0.02
O_{ij}	0.01	0.1
E_0 (0.12 fm)	1.95	0.15
E'_0 (0.12 fm)	2.25	0.15
E_0 (0.09 fm)	1.65	0.15
E'_0 (0.09 fm)	1.85	0.15
$\log \Delta E_{i+1,i}$	-1.5	0.5
$\log \Delta E'_{i+1,i}$	-1.5	0.5

- [1] E. Lunghi and A. Soni, *Phys. Lett. B* **697**, 323 (2011).
- [2] V.M. Abazov *et al.* (D0 Collaboration), *Phys. Rev. Lett.* **105**, 081801 (2010).
- [3] J. Laiho, E. Lunghi, and R. Van De Water, *Proc. Sci.*, FPCP2010 (2010) 040.
- [4] A. Lenz *et al.*, [arXiv:1203.0238](#).
- [5] E. Lunghi and A. Soni, *Phys. Rev. Lett.* **104**, 251802 (2010).
- [6] A. Lenz *et al.*, *Phys. Rev. D* **83**, 036004 (2011).
- [7] A.J. Bevan *et al.* (UTfit Collaboration), *Proc. Sci.*, ICHEP2010 (2010) 270.
- [8] A. Lenz and U. Nierste, *J. High Energy Phys.* **06** (2007) 072.
- [9] M. Bona *et al.* (UTfit Collaboration), *PMC Phys. A* **3**, 6 (2009).
- [10] T. Aaltonen *et al.* (CDF Collaboration), *Phys. Rev. D* **85**, 072002 (2012).
- [11] V.M. Abazov *et al.* (D0 Collaboration), *Phys. Rev. D* **85**, 032006 (2012).
- [12] K. Anikeev *et al.*, [arXiv:hep-ph/0201071](#).
- [13] A. Abulencia *et al.* (CDF Collaboration), *Phys. Rev. Lett.* **97**, 242003 (2006).
- [14] V.M. Abazov *et al.* (D0 Collaboration), *Phys. Rev. Lett.* **97**, 021802 (2006).
- [15] R. Aaij *et al.* (LHCb Collaboration), *Phys. Lett. B* **709**, 177 (2012).
- [16] K. Nakamura *et al.* (Particle Data Group), *J. Phys. G* **37**, 075021 (2010).
- [17] M. Bona *et al.* (UTfit Collaboration), *J. High Energy Phys.* **03** (2008) 049.
- [18] B.A. Dobrescu and G.Z. Krnjaic, *Phys. Rev. D* **85**, 075020 (2012).
- [19] W. Altmannshofer and M. Carena, *Phys. Rev. D* **85**, 075006 (2012).
- [20] A.J. Buras and J. Girrbach, *J. High Energy Phys.* **03** (2012) 052.
- [21] M. Blanke, A.J. Buras, K. Gemmler, and T. Heidsieck, *J. High Energy Phys.* **03** (2012) 024.
- [22] A.J. Buras, M. Nagai, and P. Paradisi, *J. High Energy Phys.* **05** (2011) 005.
- [23] A.J. Buras, K. Gemmler, and G. Isidori, *Nucl. Phys.* **B843**, 107 (2011).
- [24] A.J. Buras, B. Duling, T. Feldmann, T. Heidsieck, C. Promberger, and S. Recksiegel, *J. High Energy Phys.* **09** (2010) 106.
- [25] L. Wolfenstein, *Phys. Rev. Lett.* **51**, 1945 (1983).
- [26] A.J. Buras, M.E. Lautenbacher, and G. Ostermaier, *Phys. Rev. D* **50**, 3433 (1994).
- [27] F. Gabbiani, E. Gabrielli, A. Masiero, and L. Silvestrini, *Nucl. Phys.* **B477**, 321 (1996).
- [28] D. Becirevic, V. Gimenez, G. Martinelli, M. Papinutto, and J. Reyes, *J. High Energy Phys.* **04** (2002) 025.
- [29] C.M. Bouchard *et al.* (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LATTICE2011 (2011) 274.
- [30] T. Inami and C.S. Lim, *Prog. Theor. Phys.* **65**, 297 (1981); **65**, 1772(E) (1981).
- [31] A.J. Buras, M. Jamin, and P.H. Weisz, *Nucl. Phys.* **B347**, 491 (1990).
- [32] E. Gámiz, C.T.H. Davies, G.P. Lepage, J. Shigemitsu, and M. Wingate (HPQCD Collaboration), *Phys. Rev. D* **80**, 014503 (2009).
- [33] C. Albertus *et al.* (RBC and UKQCD Collaborations), *Phys. Rev. D* **82**, 014505 (2010).
- [34] R.T. Evans, A.X. El-Khadra, and M. Di Pierro (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2006 (2006) 081.
- [35] R. Evans, E. Gámiz, A.X. El-Khadra, and M. Di Pierro (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2007 (2007) 354.
- [36] R.T. Evans *et al.* (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2008 (2008) 052.
- [37] R.T. Evans *et al.* (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LAT2009 (2009) 245.
- [38] G.P. Lepage, L. Magnea, C. Nakhleh, U. Magnea, and K. Hornbostel, *Phys. Rev. D* **46**, 4052 (1992).
- [39] B. Sheikholeslami and R. Wohlert, *Nucl. Phys.* **B259**, 572 (1985).
- [40] A.X. El-Khadra, A.S. Kronfeld, and P.B. Mackenzie, *Phys. Rev. D* **55**, 3933 (1997).
- [41] E. Golowich, J. Hewett, S. Pakvasa, and A.A. Petrov, *Phys. Rev. D* **76**, 095009 (2007).
- [42] C.W. Bernard, T. Burch, K. Orginos, D. Toussaint, T.A. DeGrand, C. DeTar, S. Datta, S. Gottlieb, U.M. Heller, and R. Sugar (MILC Collaboration), *Phys. Rev. D* **64**, 054506 (2001).
- [43] M.G. Alford, W. Dimm, G.P. Lepage, G. Hockney, and P.B. Mackenzie, *Phys. Lett. B* **361**, 87 (1995).
- [44] M. Luscher and P. Weisz, *Phys. Lett.* **158B**, 250 (1985).
- [45] S. Prelovsek, *Phys. Rev. D* **73**, 014506 (2006).
- [46] C. Bernard, M. Golterman, and Y. Shamir, *Phys. Rev. D* **73**, 114511 (2006).
- [47] C. Bernard, *Phys. Rev. D* **73**, 114503 (2006).
- [48] Y. Shamir, *Phys. Rev. D* **71**, 034509 (2005).
- [49] Y. Shamir, *Phys. Rev. D* **75**, 054503 (2007).
- [50] C. Bernard, M. Golterman, and Y. Shamir, *Phys. Rev. D* **77**, 074505 (2008).
- [51] S.R. Sharpe, *Proc. Sci.*, LAT2006 (2006) 022.
- [52] A.S. Kronfeld, *Proc. Sci.*, LAT2007 (2007) 016.
- [53] M. Golterman, *Proc. Sci.*, CONFINEMENT8 (2008) 014.
- [54] G.C. Donald, C.T.H. Davies, E. Follana, and A.S. Kronfeld, *Phys. Rev. D* **84**, 054504 (2011).
- [55] C. Bernard *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **83**, 034503 (2011).
- [56] J.A. Bailey *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **79**, 054507 (2009).
- [57] C. Bernard *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **79**, 014506 (2009).
- [58] J.A. Bailey *et al.* (Fermilab Lattice and MILC Collaborations), *Proc. Sci.*, LATTICE2010 (2010) 311.
- [59] A. Bazavov *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **85**, 114506 (2012).
- [60] J.A. Bailey *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **85**, 114502 (2012).
- [61] W. Lee and S. Sharpe, *Phys. Rev. D* **60**, 114503 (1999).
- [62] C. Aubin and C. Bernard, *Phys. Rev. D* **68**, 034014 (2003).
- [63] C. Aubin and C. Bernard, *Phys. Rev. D* **68**, 074011 (2003).
- [64] S.R. Sharpe and R.S. Van de Water, *Phys. Rev. D* **71**, 114505 (2005).
- [65] C. Aubin and C. Bernard, *Phys. Rev. D* **73**, 014515 (2006).
- [66] A. Bazavov *et al.* (MILC Collaborations), *Rev. Mod. Phys.* **82**, 1349 (2010).
- [67] G.P. Lepage, *Phys. Rev. D* **59**, 074502 (1999).

- [68] K. Symanzik, *Nucl. Phys.* **B226**, 205 (1983).
- [69] G. P. Lepage and P. B. Mackenzie, *Phys. Rev. D* **48**, 2250 (1993).
- [70] Z. Hao, G. M. von Hippel, R. R. Horgan, Q. J. Mason, and H. D. Trottier, *Phys. Rev. D* **76**, 034507 (2007).
- [71] M. Wingate, J. Shigemitsu, C. T. H. Davies, G. P. Lepage, and H. D. Trottier, *Phys. Rev. D* **67**, 054505 (2003).
- [72] C. R. Allton, [arXiv:hep-lat/9610016v1](#).
- [73] L. Susskind, *Phys. Rev. D* **16**, 3031 (1977); H. S. Sharatchandra, H. J. Thun, and P. Weisz, *Nucl. Phys.* **B192**, 205 (1981).
- [74] A. S. Kronfeld, *Phys. Rev. D* **62**, 014505 (2000).
- [75] G. P. Lepage and P. B. Mackenzie, *Phys. Rev. D* **48**, 2250 (1993).
- [76] E. Gámiz, J. Shigemitsu, and H. Trottier, *Phys. Rev. D* **77**, 114505 (2008).
- [77] E. Gámiz, A. El-Khadra, and A. Kronfeld (unpublished).
- [78] Q. Mason, H. D. Trottier, C. T. H. Davies, K. Foley, A. Gray, G. P. Lepage, M. Nobes, and J. Shigemitsu (HPQCD and UKQCD Collaborations), *Phys. Rev. Lett.* **95**, 052002 (2005).
- [79] S. J. Brodsky, G. P. Lepage, and P. B. Mackenzie, *Phys. Rev. D* **28**, 228 (1983).
- [80] K. Hornbostel, G. P. Lepage, and C. Morningstar, *Phys. Rev. D* **67**, 034023 (2003).
- [81] J. L. Richardson, *Phys. Lett.* **82B**, 272 (1979).
- [82] M. Di Pierro, A. X. El-Khadra, S. Gottlieb, A. S. Kronfeld, P. B. Mackenzie, D. P. Menscher, M. B. Oktay, and J. N. Simone, *Nucl. Phys. B, Proc. Suppl.* **119**, 586 (2003).
- [83] G. P. Lepage, B. Clark, C. T. H. Davies, K. Hornbostel, P. B. Mackenzie, C. Morningstar, H. Trottier, *Nucl. Phys. B, Proc. Suppl.* **106**, 12 (2002).
- [84] C. Morningstar, *Nucl. Phys. B, Proc. Suppl.* **109**, 185 (2002).
- [85] W. Detmold and C. J. D. Lin, *Phys. Rev. D* **76**, 014501 (2007).
- [86] C. Bernard (unpublished).
- [87] C. Aubin, C. Bernard, C. DeTar, J. Osborn, S. Gottlieb, E. B. Gregory, D. Toussaint, U. M. Heller, J. E. Hetrick, and R. Sugar (MILC Collaboration), *Phys. Rev. D* **70**, 114501 (2004).
- [88] C. W. Bernard, *Phys. Rev. D* **62**, 034503 (2000).
- [89] R. Sommer, *Nucl. Phys.* **B411**, 839 (1994).
- [90] A. Bazavov *et al.* (MILC Collaboration), *Proc. Sci.*, CD09 (2009) 007.
- [91] C. T. H. Davies, E. Follana, I. D. Kendall, G. P. Lepage, and C. McNeile (HPQCD Collaboration), *Phys. Rev. D* **81**, 034506 (2010).
- [92] I. W. Stewart, *Nucl. Phys.* **B529**, 62 (1998).
- [93] R. Casalbuoni, A. Deandrea, N. Di Bartolomeo, R. Gatto, F. Feruglio, and G. Nardulli, *Phys. Rep.* **281**, 145 (1997).
- [94] A. Anastasov *et al.* (CLEO Collaboration), *Phys. Rev. D* **65**, 032003 (2002).
- [95] A. Abada, D. Becirevic, P. Boucaud, G. Herdoiza, J. P. Leroy, A. Le Yaouanc, O. Pene, and J. Rodriguez-Quintero, *Nucl. Phys. B, Proc. Suppl.* **119**, 641 (2003).
- [96] M. C. Arnesen, B. Grinstein, I. Z. Rothstein, and I. W. Stewart, *Phys. Rev. Lett.* **95**, 071802 (2005).
- [97] H. Ohki, H. Matsufuru, and T. Onogi, *Phys. Rev. D* **77**, 094509 (2008).
- [98] J. Bulava *et al.* (ALPHA Collaboration), *Proc. Sci.*, LATTICE2010 (2010) 303.
- [99] W. Detmold, C.-J. D. Lin, and S. Meinel, *Phys. Rev. D* **85**, 114508 (2012).
- [100] C. Bernard, *Proc. Sci.*, LAT2007 (2007) 090.
- [101] A. S. Kronfeld, *Nucl. Phys. B, Proc. Suppl.* **129**, 46 (2004).
- [102] M. B. Oktay and A. S. Kronfeld, *Phys. Rev. D* **78**, 014504 (2008).
- [103] W. Kilian and T. Mannel, *Phys. Lett. B* **301**, 382 (1993).
- [104] C. Bernard (MILC Collaboration), *Phys. Rev. D* **65**, 054031 (2002).
- [105] Average of the CDF and LHCb results by the Heavy Flavor Averaging Group <http://www.slac.stanford.edu/xorg/hfag/>.

Fluctuations and correlations of net baryon number, electric charge, and strangeness: A comparison of lattice QCD results with the hadron resonance gas model

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We calculate the quadratic fluctuations of net baryon number, electric charge and strangeness as well as correlations among these conserved charges in $(2 + 1)$ -flavor lattice QCD at zero chemical potential. Results are obtained using calculations with tree-level improved gauge and the highly improved staggered quark actions with almost physical light and strange quark masses at three different values of the lattice cutoff. Our choice of parameters corresponds to a value of 160 MeV for the lightest pseudoscalar Goldstone mass and a physical value of the kaon mass. The three diagonal charge susceptibilities and the correlations among conserved charges have been extrapolated to the continuum limit in the temperature interval $150 \text{ MeV} \leq T \leq 250 \text{ MeV}$. We compare our results with the hadron resonance gas (HRG) model calculations and find agreement with HRG model results only for temperatures $T \lesssim 150 \text{ MeV}$. We observe significant deviations in the temperature range $160 \text{ MeV} \lesssim T \lesssim 170 \text{ MeV}$ and qualitative differences in the behavior of the three conserved charge sectors. At $T \approx 160 \text{ MeV}$ quadratic net baryon number fluctuations in QCD agree with HRG model calculations, while the net electric charge fluctuations in QCD are about 10% smaller and net strangeness fluctuations are about 20% larger. These findings are relevant to the discussion of freeze-out conditions in relativistic heavy ion collisions.

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I. INTRODUCTION

The low energy runs currently being performed at the Relativistic Heavy Ion Collider (RHIC) [1] aim at an exploration of the QCD phase diagram at nonzero temperature (T) and baryon chemical potential (μ_B) through the measurement of fluctuations of conserved charges, e.g., net baryon number, electric charge and strangeness. For the former, first results have been published by the STAR collaboration [2] and preliminary results on the latter two have been presented at conferences. A central goal of these experiments is to search for the existence of the QCD critical point, a second order phase transition point, that has been postulated to exist at nonvanishing baryon chemical potential in the T - μ_B phase diagram of QCD [3,4]. Fluctuations in conserved charges can probe this critical point, the endpoint of a line of first order phase transitions that extends to large baryon chemical potential at nonzero quark masses. More generally, the study of fluctuations at any value of the baryon chemical potential probe thermal

conditions in a medium and provide information on the critical behavior of QCD [5].

At zero baryon chemical potential, already, the analysis of fluctuations of conserved charges and their higher order cumulants provides important information about the relation between the QCD chiral phase transition at vanishing light quark masses, the crossover temperature at physical quark masses and the freeze-out conditions observed in heavy ion experiments [5–7]. Thus, calculations of conserved charge fluctuations at $\mu_B = 0$ will provide unique information on freeze-out conditions at the LHC where the baryon chemical potential is small, $\mu_B/T \approx 0.05$. The quadratic fluctuations of the net baryon number characterize the width of the probability distribution which has been measured at RHIC [2] and has recently been analyzed in the framework of the hadron resonance gas (HRG) model [8]. Although the HRG model provides a rather satisfactory description of global hadron yields at chemical freeze-out [9], its ability to describe detailed properties of strongly

interacting matter such as fluctuations of conserved charges and, in particular, their higher order cumulants is not obvious. The foundation for the HRG model is given by the Dashen, Ma, Bernstein theorem [10], which shows that the partition function of strongly interacting matter can be described by a gas of free resonances, if the system is sufficiently dilute and the resonance production is the dominant part of the interaction among hadrons [11,12]. At very low temperature and high baryon number density, where nonresonant nucleon-nucleon interactions become important, as well as at high temperature where strongly interacting matter undergoes a transition to the quark-gluon plasma regime and partonic degrees of freedom become dominant, the HRG model is expected to be a poor approximation to the thermodynamics of strongly interacting matter. To what extent the HRG model provides a good description of strongly interacting matter needs to be explored in detail by comparing model calculations with first principal (lattice) QCD calculations. The latter provides the complete description of QCD thermodynamics at all values of the temperature and ultimately should set the standard for the interpretation of experimental results on strong interaction thermodynamics. Unfortunately, this is, at present, not fully possible. For instance, the only satisfactory way to specify the thermal conditions in a heavy ion experiment at the time of hadronization is through the comparison of experimental data with HRG model calculations [13]. It has recently been pointed out that in the future this may be overcome by comparing experimental data on conserved charge fluctuations directly with lattice QCD calculations [5]. Also in order to establish such an approach more firmly it is important to understand and quantify to what extent lattice QCD calculations and HRG model calculations agree and in which temperature regime the latter provides a reasonable approximation to strong interaction thermodynamics.

Indeed, some deviations in ratios of higher order cumulants of baryon number fluctuations, calculated within the HRG model, from experimental results for cumulants of net proton fluctuations have been observed [8]. Whether these deviations can be accounted for within QCD or are of more technical origin related to the restricted phase space in which experimental observations have been performed is an open question. In any case, a more detailed analysis of the thermal conditions achieved in heavy ion experiments is important. Lattice QCD calculations of fluctuations of conserved charges in equilibrium thermodynamics provide a base line for such discussions. Studies of fluctuations and higher order cumulants [14] may reveal differences between HRG model calculations and QCD thermodynamics that will appear close to criticality in the QCD phase diagram.

In this paper we will use the HRG model in its simplest version, i.e. as a sum of noninteracting, pointlike particles. This is known to provide an accurate description of a

dilute, strongly interacting hadron gas [11]. The need for taking into account residual interactions, for instance through the introduction of an intrinsic size of the hadrons [15] has been discussed. It has also been noted that the inclusion of higher mass resonances and an improvement in the strangeness sector of the HRG model may be needed to adequately describe pronounced features of hadron production such as the enhancement in the K/π ratio [16]. The advantage of the simplest version, however, is that the HRG model in this form is parameter free, while any improvement on this model will introduce further parameters without bringing us closer to the actual underlying theory, QCD, in a controlled way.

Quadratic fluctuations of conserved charges are closely related to quark number susceptibilities [17]. Fluctuations of net baryon number, electric charge and strangeness, as well as correlations among them, have been analyzed in previous lattice QCD calculations [18–21] and have also been used to characterize properties of the relevant thermodynamic degrees of freedom at low as well as high temperature [14,22,23]. The generic forms of their temperature dependence and their scaling properties are understood in terms of universal properties of the QCD partition function and its derivatives in the vicinity of the QCD chiral phase transition [7,20]. To make use of this knowledge in a quantitative comparison with experimental results, lattice QCD calculations close to the continuum are needed.

In this paper we present an analysis of fluctuations in, and correlations among, conserved charges using numerical calculations in $(2+1)$ -flavor QCD at three values of the lattice cutoff.¹ For these calculations we exploit an $\mathcal{O}(a^2)$ improved action consisting of a tree-level improved gauge action combined with the highly improved staggered fermion action (HISQ/tree) [26,27]. We discuss the cutoff dependence of our results in different temperature intervals and consider two different zero-temperature observables for the determination of the temperature scale used for extrapolations to the continuum limit. This allows us to quantify systematic errors in our calculation. In an appendix, we discuss the relation between temperature scales deduced from different zero-temperature observables and the propagation of their cutoff dependence into the cutoff dependence of thermodynamic observables.

II. FLUCTUATIONS OF CONSERVED CHARGES FROM LATTICE QCD: THE HADRON RESONANCE GAS AND THE IDEAL GAS LIMIT

To calculate fluctuations of baryon number (B), electric charge (Q) and strangeness (S) from (lattice) QCD we start from the QCD partition function with nonzero light (μ_u, μ_d) and strange quark (μ_s) chemical potentials.

¹Preliminary results of this work had been presented at Quark Matter 2011 [24] and PANIC 2011 [25].

The quark chemical potentials can be expressed in terms of chemical potentials for baryon number (μ_B), strangeness (μ_S) and electric charge (μ_Q),

$$\begin{aligned}\mu_u &= \frac{1}{3}\mu_B + \frac{2}{3}\mu_Q, & \mu_d &= \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q, \\ \mu_s &= \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q - \mu_S.\end{aligned}\quad (1)$$

The starting point of the analysis is the pressure p given by the logarithm of the QCD partition function,

$$\frac{p}{T^4} \equiv \frac{1}{VT^3} \ln Z(V, T, \mu_B, \mu_S, \mu_Q). \quad (2)$$

Fluctuations of the conserved charges and their correlations in a thermalized medium are then obtained from its derivatives evaluated at $\vec{\mu} = (\mu_B, \mu_Q, \mu_S) = 0$,

$$\hat{\chi}_2^X \equiv \frac{\chi_2^X}{T^2} = \frac{\partial^2 p/T^4}{\partial \hat{\mu}_X^2} \Big|_{\vec{\mu}=0}, \quad (3)$$

$$\hat{\chi}_{11}^{XY} \equiv \frac{\chi_{11}^{XY}}{T^2} = \frac{\partial^2 p/T^4}{\partial \hat{\mu}_X \partial \hat{\mu}_Y} \Big|_{\vec{\mu}=0}, \quad (4)$$

with $\hat{\mu}_X \equiv \mu_X/T$ and $X, Y = B, Q, S$. Explicit expressions for the calculation of these susceptibilities in terms of generalized light and strange quark number susceptibilities are given in [20].

As all these derivatives are evaluated at $\vec{\mu} = 0$, the expectation values of all net charge numbers $\delta N_X \equiv N_X - N_{\bar{X}}$, with N_X ($N_{\bar{X}}$), denoting the number of particles (antiparticles), vanish, i.e., $\langle \delta N_X \rangle = 0$. The susceptibilities, i.e., the quadratic fluctuations of the charges, are then given by

$$\hat{\chi}_2^X = \langle (\delta N_X)^2 \rangle / VT^3. \quad (5)$$

A. The hadron resonance gas

We will compare results for fluctuations and correlations defined by Eqs. (3) and (4) with hadron resonance gas model calculations. The partition function of the HRG model can be split into mesonic and baryonic contributions,

$$\begin{aligned}\frac{p^{\text{HRG}}}{T^4} &= \frac{1}{VT^3} \sum_{i \in \text{mesons}} \ln Z_{M_i}^M(T, V, \mu_Q, \mu_S) \\ &+ \frac{1}{VT^3} \sum_{i \in \text{baryons}} \ln Z_{M_i}^B(T, V, \mu_B, \mu_Q, \mu_S),\end{aligned} \quad (6)$$

where the partition function for mesonic (M) or baryonic (B) particle species i with mass M_i is given by

$$\begin{aligned}\ln Z_{M_i}^{M/B} &= \mp \frac{V d_i}{2\pi^2} \int_0^\infty dk k^2 \ln(1 \mp z_i e^{-\varepsilon_i/T}) \\ &= \frac{VT^3}{2\pi^2} d_i \left(\frac{M_i}{T}\right)^2 \sum_{k=1}^\infty (\pm 1)^{k+1} \frac{z_i^k}{k^2} K_2(kM_i/T).\end{aligned} \quad (7)$$

TABLE I. Ideal gas values for off-diagonal, $\hat{\chi}_{11}^{XY} \equiv \chi_{11}^{XY}/T^2$, and diagonal susceptibilities, $\hat{\chi}_2^X \equiv \chi_2^X/T^2$. Here $X, Y = B, Q, S$.

	B	Q	S
B	1/3	0	-1/3
Q	0	2/3	1/3
S	-1/3	1/3	1

Here upper signs correspond to mesons and lower signs to baryons; $\varepsilon_i = \sqrt{k^2 + M_i^2}$ denotes the energy of particle i , d_i is its degeneracy factor and its fugacity is given by

$$z_i = \exp((B_i \mu_B + Q_i \mu_Q + S_i \mu_S)/T). \quad (8)$$

With these relations it is straightforward to calculate susceptibilities and charge correlations in the HRG model using Eqs. (3) and (4).

We note that a HRG model is defined by specifying the resonance spectrum used to construct the partition function in Eq. (6). We use all hadron resonances with masses $M_H \leq 2.5$ GeV listed by the particle data group (PDG) in their 2010 summary tables² [28]. It is similar to that used, for example, in Ref. [16]. One question, that we will discuss in the comparison of lattice QCD results with HRG model calculations, is to what extent the strangeness sector is well represented in the HRG model calculations. This question has also been addressed in [16].

B. The ideal gas limit

In the infinite temperature limit, the grand canonical QCD partition function reduces to that of an ideal gas of quarks and gluons. In this limit, quark mass effects, including those in the strange quark sector, are negligible and we may compare our (2 + 1)-flavor QCD calculations with a free quark-gluon gas of 3-flavor QCD [Stefan-Boltzmann (SB) gas]. This is given by [29]

$$\frac{p_{\text{SB}}}{T^4} = \frac{8\pi^2}{45} + \frac{7\pi^2}{20} + \sum_{f=u,d,s} \left[\frac{1}{2} \left(\frac{\mu_f}{T} \right)^2 + \frac{1}{4\pi^2} \left(\frac{\mu_f}{T} \right)^4 \right], \quad (9)$$

where the first two terms give the contributions of the gluon and the quark sectors for vanishing chemical potentials. After expressing the flavor chemical potentials in terms of μ_B , μ_Q and μ_S as given in Eq. (1), it is straightforward to read off the ideal gas values for diagonal and off-diagonal susceptibilities. These are listed in Table I.

²In this summary table there are a few three starred resonances listed which do not have a known spin assignment. For these we use the minimal degeneracy factors. We also checked that the inclusion of some known heavier resonances as well as the inclusion of charmed hadrons does not alter the picture presented here. Moreover, we checked the stability of HRG results by reducing the mass cutoff from 2.5 GeV to 2.0 GeV. This alters the relevant observables discussed here by at most 2% at $T = 200$ MeV.

III. LATTICE CALCULATIONS

In order to analyze fluctuations of conserved charges, we perform calculations on gauge field configurations generated in our study of the finite-temperature transition in $(2+1)$ -flavor QCD [27]. These calculations were performed with the HISQ/tree action for three values of the lattice cutoff corresponding to lattices with temporal extent $N_\tau = 6, 8$ and 12 and a spatial lattice extent $N_\sigma = 4N_\tau$. The calculations cover a temperature range, $130 \text{ MeV} \lesssim T \lesssim 350 \text{ MeV}$. In this temperature range the line of constant physics is defined by tuning the strange quark mass m_s to its physical value and setting the light quark masses to $m_l = m_s/20$, which correspond to a pion mass $M_\pi \simeq 160 \text{ MeV}$.

It is important to note that the definition of physical quark and/or pion masses is not straightforward in calculations with staggered fermions at nonzero values of

the lattice spacing due to taste symmetry breaking. Taste symmetry breaking, which is a consequence of the doubling problem in the staggered formulation, gives rise to sixteen pseudoscalar mesons corresponding to the sixteen elements of the Clifford algebra, of which only one, with taste matrix γ_5 , behaves as a Goldstone particle at finite lattice spacing. Even in the chiral limit, the other 15 modes receive masses of $\mathcal{O}(a^2)$ which vanish only in the continuum limit. Thus, as a result of taste symmetry breaking, these sixteen modes contribute to observables with different masses. The same is true of all other states, but the problem is most severe for Goldstone modes. The size of these effects has been quantified for the staggered fermion discretization scheme exploited here (HISQ/tree) by measuring the masses of the sixteen taste pions and by defining a root-mean-squared mass [27],

$$M_\pi^{\text{rms}} = \frac{1}{4} \sqrt{M_{\gamma_5}^2 + M_{\gamma_0\gamma_5}^2 + 3M_{\gamma_i\gamma_5}^2 + 3M_{\gamma_i\gamma_j}^2 + 3M_{\gamma_i\gamma_0}^2 + 3M_{\gamma_i}^2 + M_{\gamma_0}^2 + M_1^2}. \quad (10)$$

Taste symmetry breaking also affects the generation of the ensemble of gauge configurations on which measurements are made. To simulate the desired number of flavors, the fourth-root of the staggered fermion determinant is taken for each flavor. While this “rooting” trick corrects for the number of flavors in the continuum limit, at finite lattice spacings, the masses of states contributing to the partition function are not degenerate.

With the improved staggered fermion action (HISQ/tree) used in our calculation, taste violations, while strongly suppressed, are still large [27]. In fact, our analysis showed that the HISQ/tree action has the smallest taste violations compared to the other improved staggered actions (p4, asqtad and stout) used in finite temperature calculations. Nevertheless, at values of the cutoff corresponding to the transition region ($T \simeq 160 \text{ MeV}$) on the three different N_τ lattices analyzed by us, the rms masses vary from $M_\pi^{\text{rms}} \simeq 215 \text{ MeV}$ on our finest lattices ($N_\tau = 12$) to $M_\pi^{\text{rms}} \simeq 415 \text{ MeV}$ on the coarsest lattice ($N_\tau = 6$), in contrast to the Goldstone pion mass 140 MeV [27]. We also find that, to a good approximation, the difference of M_π^{rms} and the physical pion mass M_π is proportional to the square of the lattice cutoff at a fixed value of the temperature, $(aT)^2 \sim 1/N_\tau^2$. In this paper we show that the cutoff effects resulting from a much heavier rms mass influence most strongly the electric charge fluctuations as these are most sensitive to the contributions from pions. It is worth pointing out, for comparison, that to obtain an rms mass of about 215 MeV achieved with the HISQ/tree action on $N_\tau = 12$ lattices will require $N_\tau \approx 20$ with the asqtad and stout actions [21,27].

We typically analyzed 10 000–20 000 gauge field configurations per parameter set for $N_\tau = 6$, 10 000–14 000

configurations for $N_\tau = 8$ and up to 6000 configurations for $N_\tau = 12$ lattices. Measurements of all operators needed to calculate quadratic fluctuations have been performed every 10 hybrid Monte Carlo time units for $N_\tau = 12$ and every 10 or 20 time units for $N_\tau = 6, 8$ lattices. Most of our quark number susceptibilities on the $N_\tau = 6$ and 8 lattices were calculated on Graphics Processing Unit clusters and we used 500–1500 random source vectors for the analysis. The $N_\tau = 12$ data were analyzed using 400 random source vectors at low temperatures and 100 at high temperatures.

When performing lattice QCD calculations at nonzero temperature, we have to control (at least) two different sources of cutoff errors. On the one hand there is the intrinsic cutoff dependence of the observables calculated at nonzero temperature at a certain value of the cutoff a^{-1} . We reduce these by working with tree-level $\mathcal{O}(a^2)$ improved actions in the gauge as well as the fermion sector. This improvement also insures that at high temperature the cutoff dependence of the basic operators entering our calculations is small. An additional cutoff dependence arises due to the choice of the zero temperature observable used to set the scale for all finite temperature measurements. We investigate two different scale-setting observables: the length scale r_1 extracted from the slope of the static quark potential,

$$\left(r^2 \frac{dV_{\bar{q}q}(r)}{dr} \right)_{r=r_1} = 1.0, \quad (11)$$

and the kaon decay constant f_K . The temperature in these units is $T_{r_1} r_1 = r_1/(aN_\tau)$ and $T_{f_K}/f_K = 1/(f_K a N_\tau)$. The efficacy of these observables in setting the scale is complementary in many respects [27]. In particular, we note that r_1 has a mild dependence on the quark masses and is

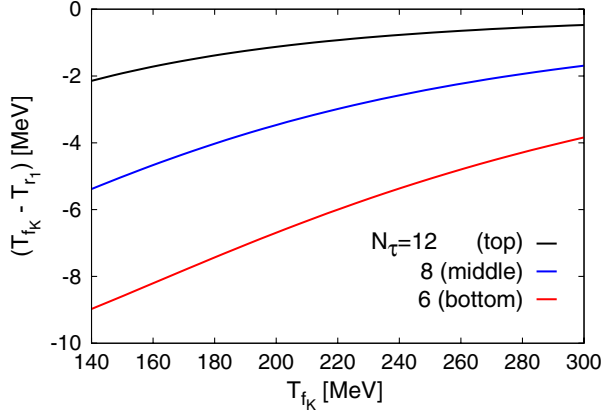


FIG. 1 (color online). Difference in temperature scales obtained from calculations of r_1 and f_K at values of the cutoff relevant for the temperature range explored in the calculation of quark number susceptibilities.

well defined even in the infinite quark mass limit. The kaon decay constant, on the other hand, has a sizeable quark mass dependence, and at lattice spacings used in this study, it is sensitive to taste symmetry violations in the hadron spectrum. To convert to physical units, we use $r_1 = 0.3106(20)$ fm [30] and the latest PDG value for the kaon decay constant, $f_K = 156.1/\sqrt{2}$ MeV. In Fig. 1, we show the difference in the two estimates of temperature over the

interval relevant to the calculations performed here. The leading order correction contributing to this difference is $\mathcal{O}(g^2 a^2)$.

As noted in [27], we also find that in the study of charge fluctuations it is advantageous to use the f_K scale as it absorbs a significant fraction of the cutoff effects, i.e., the cutoff effects are similar and cancel to a large extent in the ratio of hadron masses and temperature, M/T . However, it should be stressed that any one observable (r_1 or f_K) cannot eliminate cutoff effects in all observables equally well. We elaborate on this point in more detail in the appendix.

IV. FLUCTUATIONS

A. Fluctuations in baryon number, strangeness, and electric charge

We start our discussion of the fluctuations of baryon number, strangeness and electric charge by summarizing the data obtained on lattices with temporal extent $N_\tau = 6, 8$ and 12 in Tables II, III, and IV and discussing their scaling behavior. The continuum extrapolation and comparison to the HRG model as well as the asymptotic high temperature ideal gas results are discussed in detail in the next subsection.

Figure 2 shows results for the baryon number susceptibility with the temperature scale set using r_1 (left-hand

TABLE II. Quadratic fluctuations of net baryon number, electric charge and strangeness as well as correlations among these conserved charges in units of T^2 calculated on lattices with temporal extent $N_\tau = 6$. We use f_K to define the temperature scale.

β	T (MeV)	χ_2^B/T^2	χ_2^Q/T^2	χ_2^S/T^2	χ_{11}^{BS}/T^2	χ_{11}^{BQ}/T^2	χ_{11}^{QS}/T^2
5.900	124.17	0.0223(15)	0.1173(7)	0.0601(6)	-0.0090(6)	0.0067(6)	0.0256(2)
6.000	138.22	0.0436(28)	0.1829(12)	0.1080(10)	-0.0207(11)	0.0114(9)	0.0437(3)
6.025	141.98	0.0545(22)	0.2037(16)	0.1241(14)	-0.0258(12)	0.0144(6)	0.0491(6)
6.050	145.83	0.0590(23)	0.2283(7)	0.1426(11)	-0.0283(14)	0.0154(6)	0.0572(4)
6.075	149.79	0.0745(26)	0.2551(14)	0.1672(14)	-0.0382(13)	0.0182(6)	0.0645(5)
6.100	153.85	0.0881(24)	0.2885(14)	0.1983(14)	-0.0472(13)	0.0205(6)	0.0756(4)
6.125	158.01	0.1044(19)	0.3216(18)	0.2317(19)	-0.0580(11)	0.0225(4)	0.0868(5)
6.150	162.28	0.1256(22)	0.3614(31)	0.2741(26)	-0.0729(15)	0.0264(4)	0.1006(9)
6.175	166.66	0.1466(52)	0.3956(32)	0.3200(54)	-0.0887(29)	0.0290(25)	0.1157(20)
6.195	170.25	0.1548(32)	0.4176(20)	0.3513(30)	-0.0987(23)	0.0280(5)	0.1263(6)
6.215	173.90	0.1730(34)	0.4427(25)	0.3937(38)	-0.1155(25)	0.0288(5)	0.1391(7)
6.245	179.52	0.1881(29)	0.4666(23)	0.4422(36)	-0.1324(20)	0.0278(5)	0.1549(10)
6.285	187.27	0.2048(68)	0.4978(30)	0.5116(64)	-0.1504(50)	0.0272(32)	0.1806(31)
6.341	198.61	0.2272(20)	0.5198(24)	0.5893(40)	-0.1845(17)	0.0214(2)	0.2024(13)
6.354	201.34	0.2326(53)	0.5261(25)	0.6098(72)	-0.1936(46)	0.0195(24)	0.2083(30)
6.423	216.33	0.2517(14)	0.5466(12)	0.6881(23)	-0.2212(13)	0.0152(1)	0.2334(7)
6.488	231.33	0.2639(28)	0.5586(15)	0.7420(43)	-0.2404(26)	0.0118(13)	0.2508(18)
6.515	237.81	0.2676(9)	0.5629(9)	0.7576(17)	-0.2472(9)	0.0102(1)	0.2552(5)
6.550	246.45	0.2672(41)	0.5678(19)	0.7787(54)	-0.2528(36)	0.0072(19)	0.2629(24)
6.664	276.43	0.2777(11)	0.5714(11)	0.8101(23)	-0.2667(11)	0.0055(1)	0.2717(5)
6.800	316.10	0.2806(18)	0.5718(10)	0.8248(36)	-0.2722(18)	0.0042(8)	0.2761(14)
6.950	365.18	0.2862(27)	0.5714(15)	0.8374(57)	-0.2794(26)	0.0034(14)	0.2790(21)
7.150	440.31	0.2803(23)	0.5666(12)	0.8395(43)	-0.2783(23)	0.0010(11)	0.2804(17)

TABLE III. Same as Table II but for $N_\tau = 8$.

β	T (MeV)	χ_2^B/T^2	χ_2^Q/T^2	χ_2^S/T^2	χ_{11}^{BS}/T^2	χ_{11}^{BQ}/T^2	χ_{11}^{QS}/T^2
6.195	127.69	0.0083(58)	0.1377(19)	0.0690(13)	-0.0050(21)	0.0018(20)	0.0321(7)
6.245	134.64	0.0332(52)	0.1711(18)	0.0933(17)	-0.0151(23)	0.0090(16)	0.0391(7)
6.260	136.79	0.0390(28)	0.1868(20)	0.1054(11)	-0.0183(10)	0.0104(12)	0.0436(4)
6.285	140.45	0.0417(40)	0.2092(19)	0.1212(18)	-0.0198(20)	0.0110(11)	0.0507(3)
6.315	144.95	0.0668(38)	0.2455(23)	0.1490(31)	-0.0315(29)	0.0177(7)	0.0588(6)
6.341	148.96	0.0673(49)	0.2692(38)	0.1718(39)	-0.0345(29)	0.0164(12)	0.0686(7)
6.354	151.00	0.0705(63)	0.2908(23)	0.1878(31)	-0.0359(35)	0.0173(15)	0.0760(7)
6.390	156.78	0.0988(54)	0.3362(37)	0.2385(40)	-0.0557(31)	0.0215(11)	0.0914(10)
6.423	162.25	0.1235(28)	0.3811(15)	0.2894(23)	-0.0731(18)	0.0252(7)	0.1081(6)
6.445	165.98	0.1444(27)	0.4161(30)	0.3398(19)	-0.0919(15)	0.0263(8)	0.1239(11)
6.460	168.57	0.1610(24)	0.4287(19)	0.3623(30)	-0.1034(17)	0.0288(5)	0.1294(9)
6.488	173.49	0.1731(34)	0.4534(24)	0.4058(44)	-0.1170(28)	0.0281(4)	0.1444(10)
6.515	178.36	0.1948(24)	0.4794(28)	0.4606(35)	-0.1390(19)	0.0279(5)	0.1608(11)
6.550	184.84	0.2085(17)	0.5034(19)	0.5177(30)	-0.1572(13)	0.0257(4)	0.1803(10)
6.575	189.58	0.2190(17)	0.5171(10)	0.5586(19)	-0.1719(13)	0.0236(2)	0.1933(4)
6.608	196.01	0.2291(23)	0.5321(18)	0.6052(39)	-0.1874(22)	0.0209(1)	0.2089(10)
6.664	207.32	0.2465(22)	0.5511(13)	0.6711(35)	-0.2123(20)	0.0171(2)	0.2294(8)
6.800	237.07	0.2748(14)	0.5786(14)	0.7796(27)	-0.2540(13)	0.0104(1)	0.2628(7)
6.950	273.88	0.2901(7)	0.5963(10)	0.8443(18)	-0.2782(7)	0.0060(1)	0.2831(5)
7.150	330.23	0.2984(5)	0.6073(9)	0.8829(13)	-0.2919(5)	0.0032(1)	0.2955(4)

panel) and f_K (right-hand panel). In both cases, we show the results from the HRG model including all resonances with mass $M_H \leq 2.5$ GeV. The noticeable differences between the left and right hand panels of Fig. 2 are due to setting of the temperature scale and we find that the cutoff effects are smaller when a scale based on f_K is used. As pointed out above, this feature has also been noted in the analysis of chiral observables [27,31]. In principle, both scales should lead to identical results in the continuum limit, however, the continuum extrapolation is much better controlled when the cutoff effects are small. We therefore use the f_K temperature scale in the rest of the paper unless stated otherwise.

In Fig. 3, we show results for fluctuations of net strangeness (left) and net electric charge (right) using f_K to set the scale for the temperature. The figure also shows the corresponding HRG results. Both, the strangeness and the baryon number (see Fig. 2) fluctuations agree with HRG results for temperatures below $T \simeq 160$ MeV and show small cutoff effects. The electric charge fluctuations deviate significantly from HRG results at all temperatures and show large cutoff dependence. These large cutoff effects in $\hat{\chi}_2^Q$ can mostly be explained as due to discretization errors in the lattice hadron spectrum. The dominant contribution to $\hat{\chi}_2^Q$ at low temperatures comes from pions, while $\hat{\chi}_2^S$ receives the leading contribution from kaons and $\hat{\chi}_2^B$ from

TABLE IV. Same as Table II but for $N_\tau = 12$.

β	T (MeV)	χ_2^B/T^2	χ_2^Q/T^2	χ_2^S/T^2	χ_{11}^{BS}/T^2	χ_{11}^{BQ}/T^2	χ_{11}^{QS}/T^2
6.70	143.25	0.0404(135)	0.2741(64)	0.1586(53)	-0.0227(59)	0.0088(65)	0.0679(33)
6.74	149.03	0.0764(67)	0.3178(52)	0.1939(46)	-0.0348(40)	0.0208(32)	0.0796(25)
6.77	153.48	0.1031(68)	0.3492(86)	0.2365(59)	-0.0581(42)	0.0225(34)	0.0892(33)
6.80	158.05	0.1056(83)	0.3721(46)	0.2663(53)	-0.0632(47)	0.0212(40)	0.1015(27)
6.84	164.31	0.1520(42)	0.4358(45)	0.3531(59)	-0.0975(30)	0.0272(20)	0.1278(22)
6.88	170.77	0.1522(64)	0.4471(40)	0.3808(66)	-0.1009(46)	0.0257(30)	0.1399(30)
6.91	175.76	0.1920(46)	0.4943(36)	0.4650(63)	-0.1361(42)	0.0280(21)	0.1645(28)
6.95	182.59	0.2034(55)	0.5030(59)	0.5067(90)	-0.1506(55)	0.0264(28)	0.1780(46)
6.99	189.64	0.2273(73)	0.5273(69)	0.5779(87)	-0.1820(66)	0.0227(35)	0.1979(48)
7.03	196.91	0.2470(49)	0.5483(36)	0.6319(87)	-0.2006(45)	0.0232(24)	0.2157(34)
7.10	210.21	0.2547(33)	0.5671(27)	0.7004(106)	-0.2213(38)	0.0167(16)	0.2395(30)
7.15	220.15	0.2650(25)	0.5744(26)	0.7389(44)	-0.2366(32)	0.0142(12)	0.2512(24)
7.28	247.91	0.2822(19)	0.5902(15)	0.8063(37)	-0.2646(22)	0.0088(8)	0.2708(15)

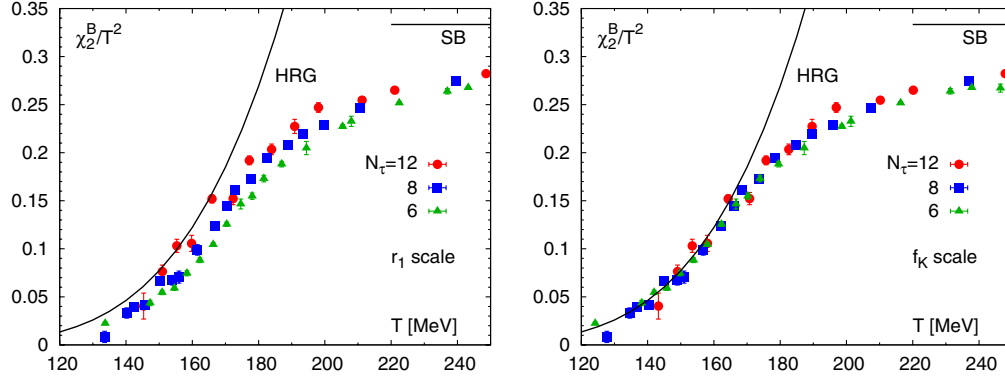


FIG. 2 (color online). Net baryon number fluctuations versus temperature. The left-hand figure shows results using the potential shape parameter r_1 to set the scale for the temperature. The right-hand figure shows the same data using f_K to set the scale. Also shown are the results obtained from the HRG model and the infinite temperature ideal gas limit (solid lines).

nucleons. As discussed in Sec. III, the pion spectrum is strongly affected by taste symmetry violations in the staggered formulation, and it has been shown in earlier work that the agreement in χ_2^O between lattice QCD results and HRG model calculations can be improved using a distorted spectrum in the HRG analysis [32,33].

To confirm this observation, we show in Fig. 3 (right panel) the HRG results obtained after replacing the physical pion mass by the rms pion mass relevant to our calculations on the $N_\tau = 6, 8$ and 12 lattices, respectively. These cutoff effects leading to the spectral distortion vary not only with N_τ but also with temperatures at fixed N_τ . We therefore parametrize the cutoff dependence of M_π^{rms} , at each N_τ , using a cubic polynomial fit to the data given in [27]. This allowed us to estimate the modified HRG result as a function of temperature, as shown in Fig. 3 by short solid lines (colored lines). The data confirm that below $T \simeq 155$ MeV, the numerical results for χ_2^O are well described by this minimally modified HRG model and the major part of the difference is indeed due to the

taste symmetry breaking effects in the pion sector. Since all other heavier states contributing to the HRG model are assumed to take on their physical values, the fluctuations of strangeness and baryon number are not influenced by this modification of the HRG model. We discuss these features, together with continuum extrapolations, for the data shown in Fig. 2 and 3 in more detail in the following subsection.

It is worthwhile to clarify our discussion of the comparison of lattice QCD data with the HRG model. When we say that the HRG is a good approximation to QCD, we refer to the value of the susceptibility, as is traditional. At the temperature where this agreement fails, we observe that not only the value but the slope also deviates significantly. Our data also indicate that the curvature starts to deviate 20–30 MeV earlier depending on the observable. These derivatives of the susceptibility are related to higher moments, which are increasingly less well captured in the HRG analysis and have not been calculated in our lattice simulations.

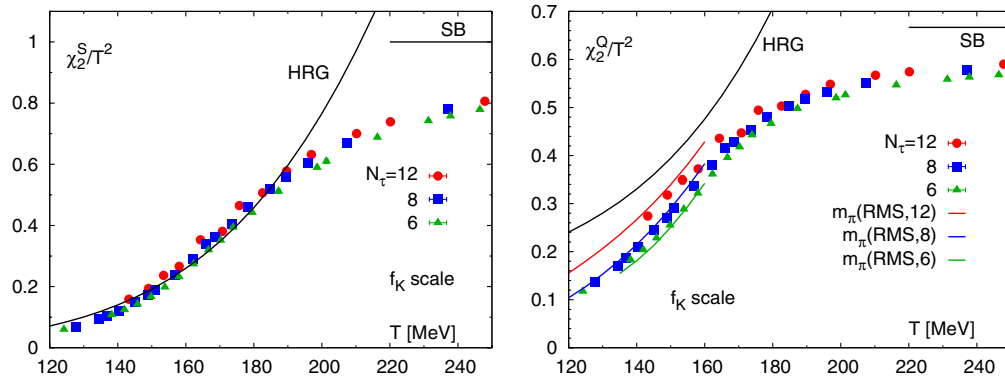


FIG. 3 (color online). Net strangeness (left) and net electric-charge (right) fluctuations versus temperature obtained from lattice calculations at three different values of the lattice cutoff $aT = 1/N_\tau$. Calculations of f_K have been used to fix the temperature scale. Also shown are the results obtained from the HRG model and the infinite temperature ideal gas limit (solid lines) as well as three short, solid lines for a HRG model in which the pion mass has been replaced by the rms pion mass relevant for our calculations on the $N_\tau = 6, 8$ and 12 lattices, respectively.

B. Continuum extrapolation and approach to the hadron resonance gas estimates

In this section, we analyze cutoff effects at fixed values of the temperature for three values of the lattice spacing, $aT = 1/6$, $1/8$ and $1/12$. We perform this analysis for temperature scales defined in terms of both r_1 and f_K in order to quantify systematic effects at a given lattice spacing and to demonstrate consistency between the estimates in the continuum limit. Our simulations on the lattices with the three different N_τ values have not been done at the same values of the temperature. As a result, in order to perform continuum extrapolations at fixed temperature, we have used cubic spline interpolations of our data throughout this paper. We propagate errors on the spline parameters.

In addition to estimating statistical errors based on our entire data sample, we also use the difference of spline interpolations performed on two independent subsets constructed by choosing every second T -point (even and odd points), as an estimate for the systematic errors. The final error on our data is obtained by adding this error estimate

and the purely statistical error obtained from the full data set in quadrature.

We first discuss the continuum extrapolation for the three susceptibilities shown in Figs. 2 and 3 at high temperature, $T \geq 170$ MeV. In this regime, cutoff effects are generally small, which, to some extent, is due to the fact that our numerical calculations have been performed with an $\mathcal{O}(a^2)$ improved action with small cutoff dependence of thermodynamic observables in the infinite temperature ideal gas limit [34]. In Fig. 4, we show continuum extrapolations for all three susceptibilities, $\chi_2^{S,Q,B}$, at three representative values of the temperature, $T = 170, 190$ and 210 MeV. In each case, and for both temperature scales, r_1 and f_K , the fits show that the cutoff effects are consistent with $\mathcal{O}(g^2(aT)^2)$ corrections and, over the limited range of T , all three susceptibilities can be extrapolated to the continuum with an Ansatz that includes corrections linear in $1/N_\tau^2 = (aT)^2$. The continuum extrapolated results obtained with the two temperature scales agree within errors, and the results obtained on the $N_\tau = 12$ lattices are a good approximation to these.

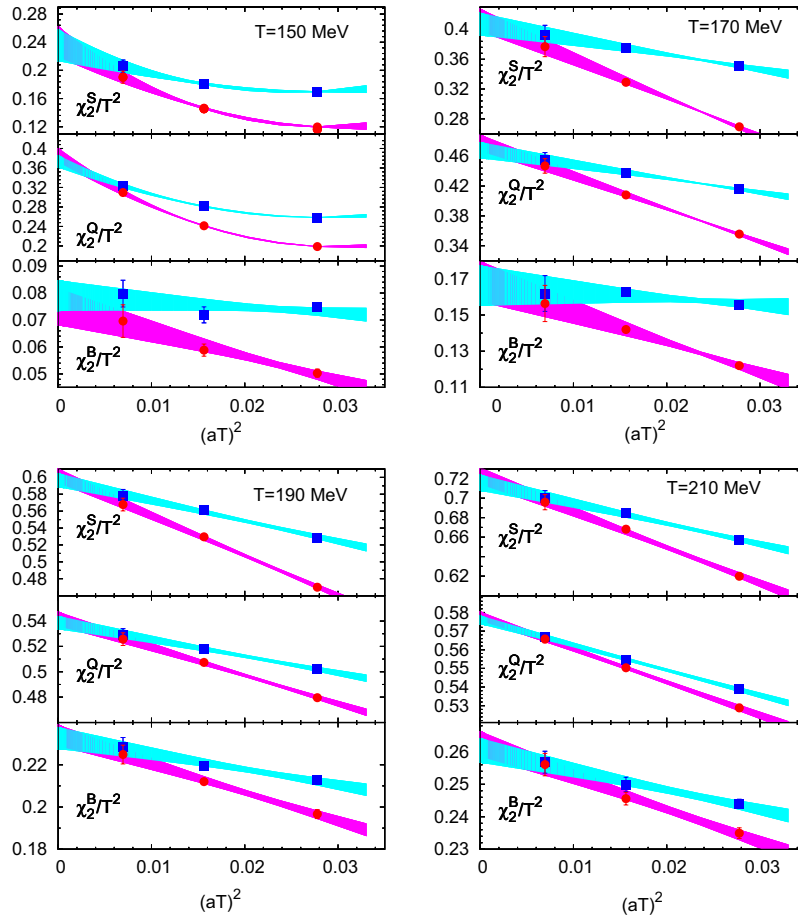


FIG. 4 (color online). Continuum extrapolations of net strangeness (χ_2^S/T^2), net electric charge (χ_2^Q/T^2) and net baryon number (χ_2^B/T^2) at four values of the temperature using fits linear and, for χ_2^S/T^2 and χ_2^Q/T^2 , at the lowest temperature quadratic in $(aT)^2 = 1/N_\tau^2$. Data at fixed values of the temperature are obtained from cubic spline interpolations. The temperature scale has been determined using calculations of r_1 (circles) and f_K (boxes), respectively.

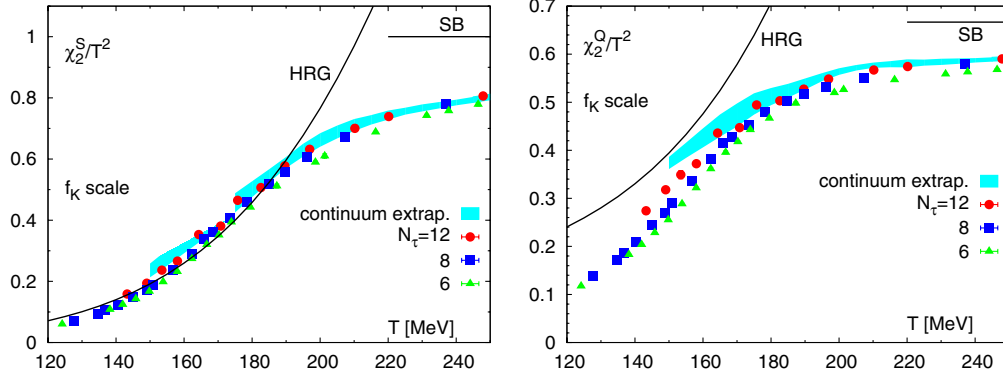


FIG. 5 (color online). Fluctuations of net strangeness (left) and electric charge (right) in units of T^2 . Calculations of f_K have been used to fix the temperature scale. Also shown are continuum extrapolated results taking into account cutoff effects up to quadratic order in $1/N_\tau^2$. The HRG model result and the SB limit is given by the solid lines.

This also is true for lower temperatures. However, in this case extrapolations linear in $1/N_\tau^2$ are no longer sufficient for the electric charge and strangeness fluctuations. Systematic effects at $\mathcal{O}((aT)^4)$ start to become important. This is evident from the data sets at $T = 150$ MeV, which are shown in Fig. 4 as well. We note that also at this temperature, which is the lowest temperature for which we perform continuum extrapolations, extrapolations based on the r_1 and f_K temperature scales are in good agreement.

Having demonstrated consistency of the continuum estimate obtained using r_1 and f_K , we, as stated previously, use the scale from f_K in the rest of the paper because the slope in the fits is smaller.

The data for the net charge fluctuations in the temperature interval 120–250 MeV, results of the linear extrapolation for χ_2^B/T^2 , and quadratic extrapolations for χ_2^S/T^2 and χ_2^Q/T^2 are shown in Figs. 5 and 6. In Fig. 6 (right) we also show the ratio of net baryon number and electric charge fluctuations. The continuum extrapolation shown for this quantity has been obtained from the corresponding extrapolations for χ_2^B/T^2 and χ_2^Q/T^2 .

Continuum extrapolations in the crossover and the low temperature regions require additional considerations because the three different conserved charge susceptibilities show different sensitivities to cutoff effects. In order to quantify differences from the HRG model results in this temperature regime, and in order to clarify the extent to which the HRG model provides a good description of QCD results, we analyze the ratios $\chi_2^X/\chi_2^{X,\text{HRG}}$, $X = B, Q$, and S , in Fig. 7. We find that, while baryon number fluctuations start to agree with HRG model results for $T \lesssim 165$ MeV, the net strangeness fluctuations become larger than the HRG values for temperatures below $T \approx 190$ MeV and then approach the HRG values from above at $T \lesssim 150$ MeV. At $T \sim 150$ MeV, the differences are still (10%–20)%.

The electric charge fluctuations show much larger deviations from the HRG model as is evident from Fig. 7. In particular, below $T \approx 170$ MeV, the cutoff dependence in $\chi_2^Q/\chi_2^{Q,\text{HRG}}$ is large and extrapolations including just leading order a^2 -corrections fail. As discussed in Sec. IVA, this, to a large extent, is due to the severe cutoff dependence of the pion spectrum, i.e., the anomalously large rms

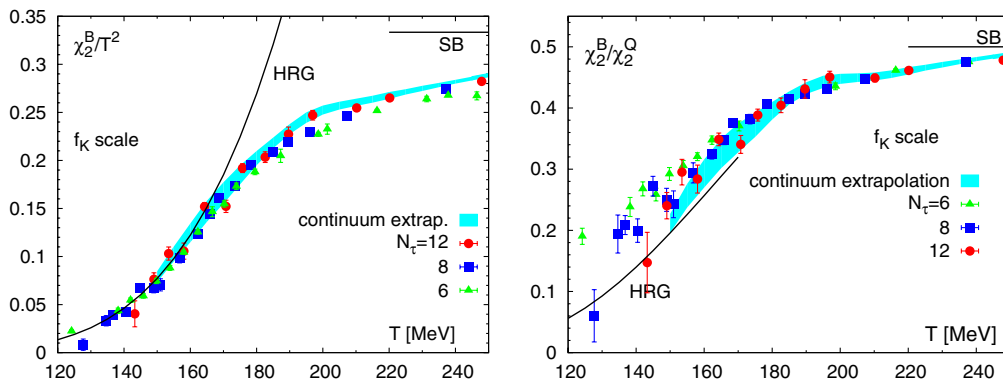


FIG. 6 (color online). Net baryon number fluctuations in units of T^2 (left) and the ratio of net baryon number and net electric charge fluctuations (right). Calculations of f_K have been used to fix the temperature scale. Also shown are results from a continuum extrapolation taking into account $\mathcal{O}(a^2)$ corrections. For χ_2^B/χ_2^Q we also show the ratio of continuum extrapolations constructed for χ_2^B/T^2 and χ_2^Q/T^2 separately. The HRG model result and the SB limit is given by the solid lines.

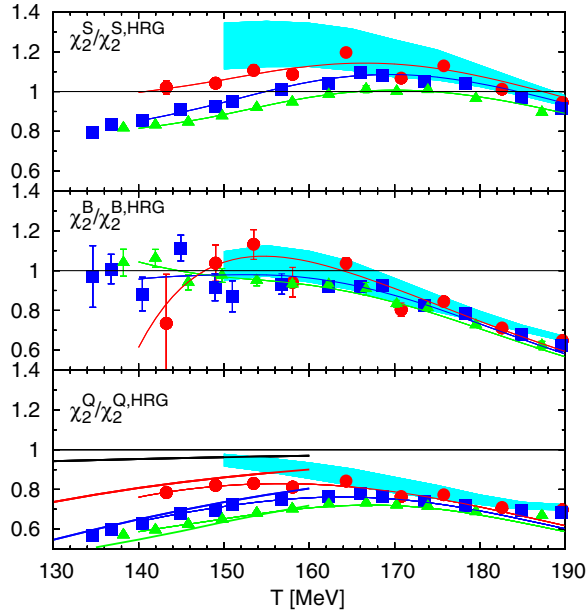


FIG. 7 (color online). Deviations of $\chi_2^{S,B,Q}$ from HRG model results. Data on $N_\tau = 6, 8$ and 12 lattices are shown using triangles, boxes and circles, respectively. Thin lines are the result of a cubic spline interpolation of the data at fixed N_τ . The broad bands are the result of the continuum extrapolations. In the bottom panel, the thick black line just below unity is the ratio $\text{HRG}(M_\pi = 160 \text{ MeV})/\text{HRG}(M_\pi^{\text{physical}})$. The other thick lines show the ratio $\text{HRG}(M_\pi^{\text{rms}})/\text{HRG}(M_\pi^{\text{physical}})$ for each of the three N_τ lattices.

pion mass suppresses fluctuations in the electric charge and has a much smaller effect on the baryon and strangeness charges. In short, a continuum extrapolation without including the effects of taste symmetry breaking is insufficient.

The distorted HRG model, which modifies the log of the partition function by replacing M_π by M_π^{rms} in the pion contribution, $\exp(-M_\pi/T)$, however, does describe the data well. In general, the HRG model defined in Eq. (7) suggests that, in this temperature regime, cutoff effects in any quantity f may be accounted for by an exponential Ansatz of the form

$$f(N_\tau, T) = a(T) + b(T)e^{-c(T)/N_\tau^2}, \quad (12)$$

which, at high temperatures where cutoff effects become small, reduces to the linear fit in $1/N_\tau^2$, i.e., $f(N_\tau, T) \approx \tilde{a}(T) + \tilde{b}(T)/N_\tau^2$ and also incorporates the next to leading order quadratic corrections $f(N_\tau, T) \approx \tilde{a}(T) + \tilde{b}(T)/N_\tau^2 + \tilde{c}(T)/N_\tau^4$.

We, therefore, analyze our data for $\hat{\chi}_2^{Q,S}$ in the transition region, $150 \leq T \leq 190$ MeV, from the low to high temperature phase of $(2+1)$ -flavor QCD using fits linear and quadratic in $1/N_\tau^2$ as well as the exponential Ansatz given in Eq. (12). With our current statistical accuracy we are, however, not sensitive to cutoff effects beyond $\mathcal{O}((aT)^4)$.

In fact, all our fits performed with the exponential ansatz are consistent within errors with fits based on the quadratic ansatz. We, therefore, do not discuss the exponential fits any further in this paper. In the case of $\hat{\chi}_2^B$ we find that linear and quadratic fits agree within errors and lead to a χ^2/dof less than unity in the entire range of temperatures $T \geq 150$ MeV. We therefore use the linear fits to perform continuum extrapolations for $\hat{\chi}_B$. For strangeness and electric charge susceptibilities we use quadratic extrapolations in the entire temperature range, although, as discussed above, we do not observe systematic differences between linear and quadratic extrapolations for $T \geq 170$ MeV. Using the latter for our continuum extrapolations, however, leads to more conservative error estimates.

A summary of our continuum extrapolations for $\chi_2^X/\chi_2^{X,\text{HRG}}$ and the data in the low temperature region is also shown in Fig. 7. Because of taste symmetry breaking, the data show significant dependence on N_τ for $T \leq 170$ MeV. To understand this cutoff effect we compare, in the bottom panel in Fig. 7, results for $\chi_2^Q/\chi_2^{Q,\text{HRG}}$ with a modified HRG model in which the physical pion mass is replaced by (i) the N_τ dependent rms mass, $\text{HRG}(M_\pi^{\text{rms}})/\text{HRG}(M_\pi^{\text{physical}})$, and (ii) a pion mass of 160 MeV, $\text{HRG}(M_\pi = 160 \text{ MeV})/\text{HRG}(M_\pi^{\text{physical}})$, corresponding to the light quark mass actually used in our calculations. Since the line showing $\text{HRG}(M_\pi = 160 \text{ MeV})/\text{HRG}(M_\pi^{\text{physical}})$ is much closer to unity compared to the other three, we confirm that the errors due to simulating at this slightly heavier pion mass are significantly smaller than the cutoff effects leading to a much heavier rms mass.

In the interesting temperature range relevant to the discussion of freeze-out conditions in heavy ion collisions, $160 \text{ MeV} \leq T \leq 170 \text{ MeV}$, we find that the continuum extrapolated electric charge fluctuations are (10–20)% smaller than even the modified HRG model calculation with $M_\pi = 160 \text{ MeV}$. For temperatures $T \leq 150$ MeV, the χ_2^Q data start to agree with the modified HRG results with $M_\pi = M_\pi^{\text{rms}}$ and continuum extrapolations using the quadratic Ansatz start to agree with the HRG result.

Strangeness fluctuations on the other hand, both for the $N_\tau = 12$ data and the continuum extrapolated values, stay systematically above the hadron resonance gas result in the temperature range 150–190 MeV. We, therefore, expect this feature to survive the continuum extrapolation. Below $T \leq 150$ MeV, fluctuations in the strangeness charge show an N_τ dependence, which is most likely again due to taste symmetry violations. More data are required to study this issue further.

Net baryon number fluctuations are consistent with HRG model results for temperatures below $T \approx 160$ MeV, although statistical errors on our $N_\tau = 12$ data set make the quantification of possible deviations from the HRG result in this temperature range difficult. For larger

TABLE V. Continuum extrapolated results for the quadratic fluctuations of net baryon number, electric charge and strangeness densities and the correlations among them. Results for χ_2^Q/T^2 and χ_2^S/T^2 are obtained from quadratic fits and those for χ_2^B/T^2 from linear fits.

T [MeV]	χ_2^B/T^2	χ_2^Q/T^2	χ_2^S/T^2	χ_{11}^{BS}/T^2	χ_{11}^{BQ}/T^2	χ_{11}^{QS}/T^2
150	0.0790(57)	0.3736(126)	0.2358(225)	-0.0415(60)	0.0187(29)	0.0929(61)
155	0.1026(77)	0.3998(158)	0.2770(260)	-0.0587(69)	0.0221(24)	0.1031(68)
160	0.1247(98)	0.4258(198)	0.3208(289)	-0.0767(75)	0.0242(23)	0.1173(70)
165	0.1470(109)	0.4513(232)	0.3645(322)	-0.0949(81)	0.0259(21)	0.1332(78)
170	0.1662(111)	0.4734(240)	0.4067(334)	-0.1115(84)	0.0269(21)	0.1491(84)
175	0.1849(99)	0.4964(222)	0.4567(314)	-0.1304(79)	0.0270(19)	0.1655(83)
180	0.2024(74)	0.5118(179)	0.5013(259)	-0.1497(66)	0.0263(17)	0.1782(77)
185	0.2182(56)	0.5239(144)	0.5449(215)	-0.1682(57)	0.0249(19)	0.1892(76)
190	0.2326(52)	0.5379(115)	0.5888(181)	-0.1860(56)	0.0233(22)	0.2005(72)
195	0.2445(55)	0.5522(84)	0.6289(210)	-0.2005(60)	0.0220(21)	0.2122(68)
200	0.2524(46)	0.5638(68)	0.6623(222)	-0.2116(52)	0.0205(21)	0.2235(70)
205	0.2570(41)	0.5717(57)	0.6884(210)	-0.2200(38)	0.0186(18)	0.2335(67)
210	0.2604(38)	0.5770(55)	0.7113(194)	-0.2267(31)	0.0168(15)	0.2424(62)
215	0.2637(36)	0.5792(63)	0.7282(155)	-0.2335(32)	0.0152(14)	0.2486(51)
220	0.2676(35)	0.5809(84)	0.7438(148)	-0.2397(35)	0.0140(12)	0.2537(57)
225	0.2713(28)	0.5824(63)	0.7565(113)	-0.2456(34)	0.0128(12)	0.2576(56)
230	0.2749(27)	0.5841(64)	0.7672(116)	-0.2511(33)	0.0119(12)	0.2606(56)
235	0.2784(23)	0.5855(56)	0.7760(105)	-0.2564(28)	0.0109(10)	0.2628(48)
240	0.2819(20)	0.5873(46)	0.7847(92)	-0.2613(24)	0.0101(8)	0.2649(39)
245	0.2852(20)	0.5890(45)	0.7934(98)	-0.2664(23)	0.0093(8)	0.2667(37)
250	0.2885(20)	0.5907(45)	0.8020(98)	-0.2710(23)	0.0085(7)	0.2688(34)

values of the temperature, the estimates and errors in them grow progressively smaller. Our linear extrapolations suggest that in the temperature interval $160 \text{ MeV} \leq T \leq 170 \text{ MeV}$, deviations from the HRG model calculations are at most 10%. A confirmation of this in our data, through the inclusion of quadratic corrections, however, requires better statistics. Data obtained with the stout action [21] also suggest that the χ_2^B stays close to the HRG model result in this temperature range.

In order to reflect the influence of systematic effects on our continuum extrapolation we varied fit ranges and distribution of knots in the smooth spline interpolation. Moreover, in order to account for possible underestimates of errors on the individual data points, we divided our data samples into two independent subsets consisting of even and odd T -values by rank-order. We used the differences in these fits and the fit to the full data sample as an additional error on our spline interpolations.

To summarize, our continuum extrapolated values of $\chi_2^{B,Q,S}/T^2$ are given in Table V. Extrapolations of $\chi_2^{Q,S}/T^2$ used the Ansatz, Eq. (12) truncated at $O(1/N_\tau^4)$, i.e., we used the quadratic extrapolations, whereas for χ_2^B/T^2 the exponential was truncated at $O(1/N_\tau^2)$, i.e., we used the linear extrapolations. For $\chi_2^{Q,S}/T^2$ we also find that the quadratic extrapolated values agree with the exponential Ansatz. Our extrapolated results are in good agreement with the recently published analysis using the stout action [21].

Lastly, in Fig. 6 (right), we show the ratio of the net baryon number and electric charge fluctuations, χ_2^B/χ_2^Q . It approaches the HRG model result from above and starts to agree with it for $T \leq 150 \text{ MeV}$. The continuum extrapolation here is based on the linear and exponential extrapolations for χ_2^B and χ_2^Q , respectively. In the region of interest to heavy ion phenomenology, this ratio varies between 0.29(4) (at 160 MeV) and 0.35(4) (170 MeV). Thus, fluctuations in net electric charge could be 3–4 times larger than in the net baryon number in the vicinity of the freeze-out temperature.

V. CORRELATIONS

Probes of the structure of QCD at finite temperature include correlations among different conserved charges. These correlations show characteristic changes in the crossover region between the low and high temperature phases of QCD, which are correlated with changes in the relevant degrees of freedom. They also provide insight into the applicability of HRG model calculations at low temperatures. The change in correlations between baryon number and electric charge, χ_{11}^{BQ} , is expected to be particularly striking as one goes from the low to the high temperature phase. At low temperatures this correlation is dominated by the contribution of protons plus antiprotons. Consequently, within the HRG model it rises exponentially with temperature in this region. In the high

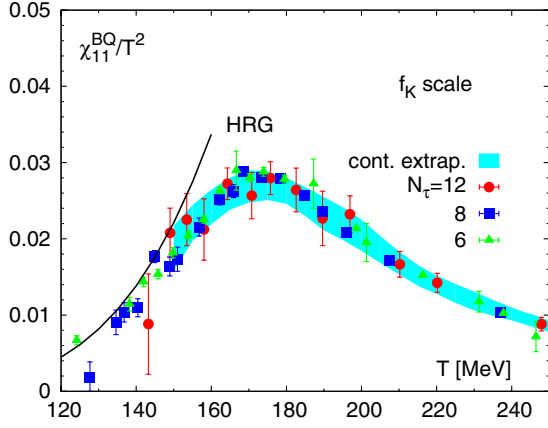


FIG. 8 (color online). Correlations of electric charge with baryon number versus temperature. The temperature scale has been set using f_K . The solid line shows the result for the HRG model. The band shows continuum extrapolations that take into account cutoff effects linear in $1/N_\tau^2$.

temperature limit of $(2+1)$ -flavor QCD, however, $\hat{\chi}_{11}^{BQ}$ vanishes as the quarks become effectively massless, ($m_i/T \rightarrow 0$), and the weighted sum of the charges of up, down and strange quarks vanishes. Results for $\hat{\chi}_{11}^{BQ}$ shown in Fig. 8 are consistent with this picture.

The correlations of strangeness with the baryon number and the electric charge, $\hat{\chi}_{11}^{BS}$ and $\hat{\chi}_{11}^{QS}$, are sensitive to changes in the strangeness degrees of freedom [22,35,36]. Results for the temperature dependence of these correlations are shown in Fig. 9. They approach the Stefan-Boltzmann value, $1/3$, of a massless three flavor quark gas at high temperatures. As observed in the case of the quadratic fluctuations, on decreasing the temperature toward the transition region, these correlations first overshoot the HRG model result and then approach HRG value from above at about 150 MeV. This overshoot is more pronounced for $-\hat{\chi}_{11}^{BS}$ than for $\hat{\chi}_{11}^{QS}$.

Also shown in Fig. 9 are continuum extrapolations (bands) which in the baryon sector, i.e., for B-S and B-Q

correlations, are based on fits linear in $1/N_\tau^2$, whereas in the meson sector, i.e., for Q-S correlations, quadratic corrections are also taken into account. This reflects the larger sensitivity of the latter to taste violations that also has been observed for the quadratic strangeness and electric charge fluctuations.

In the isospin symmetric case considered in this study, the flavor correlations $\hat{\chi}_{11}^{us}$ and $\hat{\chi}_{11}^{ds}$ are equal. Also, the two correlations $2\hat{\chi}_{11}^{QS}$ and $\hat{\chi}_{11}^{BS}$ are related to each other through the quadratic strangeness fluctuations, i.e., $2\hat{\chi}_{11}^{QS} - \hat{\chi}_{11}^{BS} = \hat{\chi}_2^s$ [36]. One can then write the following relationships between the charge correlations and quark-flavor fluctuations:

$$\hat{\chi}_{11}^{QS} = \frac{1}{3}(\hat{\chi}_2^s - \hat{\chi}_{11}^{us}), \quad \hat{\chi}_{11}^{BS} = -\frac{1}{3}(\hat{\chi}_2^s + 2\hat{\chi}_{11}^{us}). \quad (13)$$

At high temperatures $\hat{\chi}_{11}^{QS} \sim -\hat{\chi}_{11}^{BS}$ because $\hat{\chi}_{11}^{us}$ receives perturbative contributions only at $\mathcal{O}(g^6 \ln(1/g^2))$ and is therefore small [23,37]. On the other hand, corrections to $\hat{\chi}_2^s$ from the ideal gas limit are dominant as they are $\mathcal{O}(g^2)$.

All three charge correlations show significant deviations from the ideal gas limit even at twice the transition temperature (see data in Tables II, III, and IV). These deviations are due to large contributions of flavor fluctuations, such as to $\hat{\chi}_2^s$ discussed above. The leading order perturbative correction can be eliminated by forming suitable ratios that can be used to analyze experimental data on charge fluctuations [22,35,36],

$$C_{BS} = -3 \frac{\chi_{11}^{BS}}{\chi_2^s}, \quad C_{QS} = 3 \frac{\chi_{11}^{QS}}{\chi_2^s} = \frac{1}{2}(3 - C_{BS}). \quad (14)$$

At high temperature the deviations from the ideal gas value of unity are now due to χ_{11}^{us}/χ_2^s , for example, $C_{BS} = 1 + 2\chi_{11}^{us}/\chi_2^s$. Data for C_{BS} is shown in Fig. 10 (left) and, in comparison to the quadratic strangeness fluctuations (Fig. 3) or baryon number strangeness correlations (Fig. 9), the approach to the ideal gas limit is much more

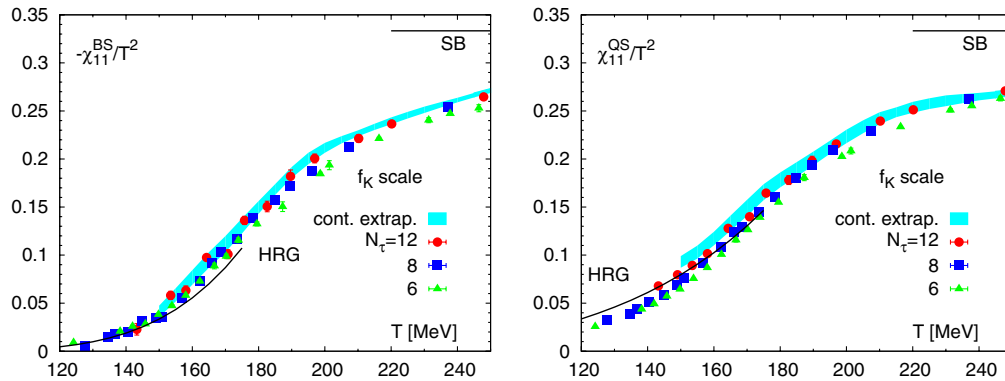


FIG. 9 (color online). Correlations of strangeness with baryon number (left) and electric charge (right). In both cases, f_K has been used to set the scale. The solid lines show the result for the HRG model. For χ_{11}^{BS}/T^2 the band shows continuum extrapolations that take into account cutoff effects linear in $1/N_\tau^2$ while for χ_{11}^{QS}/T^2 also quadratic corrections have been accounted for.

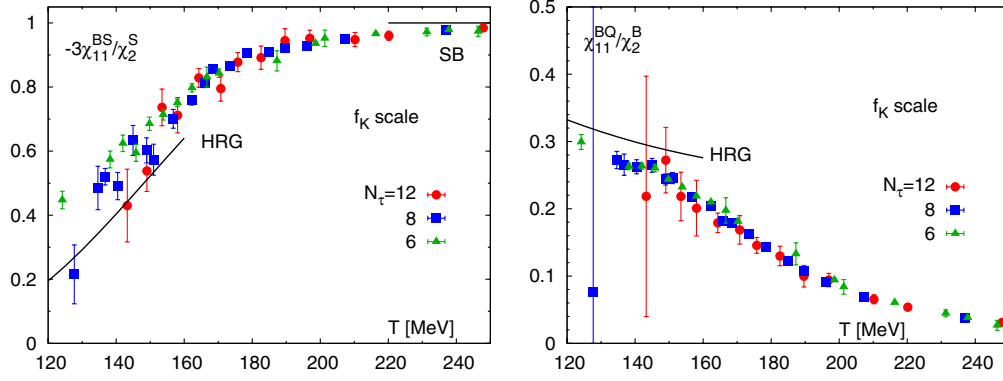


FIG. 10 (color online). Correlations between baryon number and strangeness (left) as well as electric charge (right) normalized to strangeness and net baryon number fluctuations, respectively. The solid line shows the HRG model result.

rapid. This shows that the flavor correlation $2\chi_{11}^{us}/\chi_2^s$ is already small for $T \gtrsim 1.2T_c$. It is, however, large in the vicinity of the transition temperature.

The behavior of the third ratio that one can analyze, $C_{BQ} = \chi_{11}^{BQ}/\chi_2^B$, is somewhat different as leading order perturbative corrections do not cancel completely due to differences in the light and strange quark masses. Consequently, the approach to the ideal gas limit is slower as can be seen in Fig. 10 (right).

VI. DISCUSSION AND CONCLUSION

We have analyzed quadratic fluctuations and correlations among conserved charges in $(2+1)$ -flavor QCD. We find that as the temperature is decreased from the high temperature phase, the net baryon number fluctuations start to agree with the hadron resonance gas model below 165 MeV while for electric charge fluctuations this happens only below 150 MeV. The fluctuations of net strangeness overshoot the HRG model values at $T \sim 190$ MeV. In the temperature range relevant to the discussion of chemical freeze-out in heavy ion collisions, 160–170 MeV, strangeness fluctuations are systematically larger than the HRG model result by about 20%. These detailed differences between QCD calculations and HRG model results should become manifest when experimental data on the probability distributions of net charge fluctuations [2] is analyzed.

In fact, quadratic fluctuations characterize the bulk structure of these distributions which, in the Gaussian approximation at $\mu_B = 0$, is given by

$$P(N_X) = e^{-N_X^2/(2V_f T_f^3 \hat{\chi}_2^X)}, \quad X = B, S, Q, \quad (15)$$

where T_f denotes the temperature at the time of chemical freeze-out and V_f is the freeze-out volume. The results presented here suggest that the largest deviations from HRG model calculations occur in the probability distributions for electric charge and strangeness fluctuations. We give a summary of the fluctuations in conserved charges for temperatures in the transition region in Table VI.

In the phenomenologically interesting temperature regime $160 \text{ MeV} \lesssim T \lesssim 170 \text{ MeV}$, continuum extrapolated results for $\hat{\chi}_2^Q$, are smaller than the HRG model results by about 10%–20%. Even though at temperatures below 150 MeV, estimates for electric charge fluctuations have large systematic errors due to the distortion of the light meson spectrum in all staggered formulations, our analysis shows that these effects can be taken into account when performing continuum extrapolations. We show that the resulting continuum estimates in the transition region lie below the HRG estimates even after corrections accounting for the distorted pion spectrum have been applied. Thus, our conclusion is that at the highest RHIC energies and at the LHC, the width of probability

TABLE VI. Quadratic fluctuations of net baryon number (δN_B), electric charge (δN_Q) and strangeness (δN_S) densities and correlations among these conserved net charges in the crossover region from the low to high temperature regime of QCD. We give results for quadratic fluctuations and correlations calculated in QCD relative to the corresponding HRG model results.

T [MeV]	$\chi_2^B/\chi_2^{B,HRG}$	$\chi_2^Q/\chi_2^{Q,HRG}$	$\chi_2^S/\chi_2^{S,HRG}$	$\chi_2^{BS}/\chi_2^{BS,HRG}$	$\chi_2^{BQ}/\chi_2^{BQ,HRG}$	$\chi_2^{QS}/\chi_2^{QS,HRG}$
155	1.049(79)	0.924(36)	1.240(116)	1.353(159)	0.804(86)	1.139(74)
160	1.020(80)	0.895(41)	1.235(111)	1.384(135)	0.717(67)	1.144(68)
165	0.972(72)	0.861(44)	1.212(106)	1.356(116)	0.633(51)	1.150(67)
170	0.898(60)	0.818(41)	1.171(96)	1.280(96)	0.544(42)	1.144(64)

distribution for the net electric charge should be narrower than what HRG model calculations would suggest since $\hat{\chi}_2^Q$ in Eq. (15) is smaller.

In the case of the net baryon number fluctuations, deviations from HRG model results start to become statistically significant only for $T \gtrsim 165$ MeV and will therefore be hard to quantify. We also find that the ratio of the net baryon number and electric charge fluctuations, presented in Fig. 6, approaches the HRG model result from above and starts to agree with it for $T \lesssim 150$ MeV. In the transition region this ratio is

$$\frac{\chi_2^B}{\chi_2^Q} \approx (0.29-0.35) \text{ for } 160 \text{ MeV} \leq T \leq 170 \text{ MeV}, \quad (16)$$

i.e., fluctuations in net electric charge are expected to be about three to four times larger in the vicinity of the freeze-out temperature in heavy ion collisions than net baryon number fluctuations. It is worth noting that a comparison of χ_2^B/χ_2^Q with the ratio of proton to net charge fluctuations, which is accessible in heavy ion collisions, will allow us to relate fluctuations in the proton number to the fluctuations of the conserved net baryon number [38].

Finally, we point out that the continuum extrapolated results presented here, and summarized in Table VI in a temperature regime relevant to the freeze-out conditions in heavy ion collisions, do not rely on any uncertainties in the determination of the QCD crossover temperature or its characterization through different observables as discussed in [27]. Systematic errors on the temperature values listed in the first row of Table VI can only come from uncertainties in the zero-temperature observable used to determine the temperature scale. We estimate these uncertainties to be less than 2 MeV in our calculation [27].

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APPENDIX: CHOICE OF TEMPERATURE SCALE AND THE HADRON SPECTRUM

In this Appendix we discuss the effect of setting the scale using different observables with mass-dimension one calculated in zero-temperature simulations. We denote lattice observables measured in units of the lattice spacing and calculated at a given β by $O_i(\beta)$. In the limit $\beta \equiv 10/g^2 \rightarrow \infty$, these approach their physical value O_i^{phy} as

$$O_i(\beta) = \frac{O_i^{\text{phy}}}{\Lambda_L} R(\beta)(1 + g^2 b_i R^2(\beta)), \quad (A1)$$

where Λ_L is the QCD scale, $R(\beta) \equiv a(\beta)\Lambda_L$ is the β -function, and only the leading correction $\mathcal{O}(g^2 a^2)$, relevant to our tree-level improved staggered formulation, has been retained.

Consider using the observable O_i to define the temperature scale T_i . On a lattice of temporal size N_τ , this temperature is given in terms of O_i^{phy} as

$$T_i(\beta) = \frac{O_i^{\text{phy}}}{O_i(\beta)N_\tau}. \quad (A2)$$

The ratio of any two such temperature scales is then given by

$$\begin{aligned} \frac{T_1(\beta)}{T_2(\beta)} &= \frac{O_1^{\text{phy}}}{O_1(\beta)} \frac{O_2(\beta)}{O_2^{\text{phy}}} = \frac{1 + b_2 g^2 R^2(\beta)}{1 + b_1 g^2 R^2(\beta)} \\ &\approx 1 + (b_2 - b_1) g^2 R^2(\beta). \end{aligned} \quad (A3)$$

Using Eqs. (A2) and (A3) we can express the observable $O_2(\beta)$ in terms of the temperature scale T_1 obtained from O_1 as

$$O_2(\beta)N_\tau = \frac{O_2^{\text{phy}}}{T_2} \approx \frac{O_2^{\text{phy}}}{T_1} (1 + (b_2 - b_1) g^2 R^2(\beta)). \quad (A4)$$

This shows that if an observable of interest (O_2) has a cutoff dependence similar to that of observable (O_1) used to determine the temperature scale T_1 , i.e., $b_2 \approx b_1$, then $O_2(\beta)N_\tau$, as an estimate of O_2^{phy}/T_1 , has small cutoff effects. Since all the $b_i - b_1$ need not be small, improving the scaling behavior of one observable does not, in general, imply improvement in all observables.

In the low temperature regime of QCD, the relevant degrees of freedom are hadrons with masses M_H . If the hadron resonance gas is a good approximation in this regime, continuum extrapolations of lattice data are better controlled if a temperature scale is chosen such that all the lattice estimates of M_H/T have small cutoff

dependences. We find that using a hadronic observable such as f_K improves the scaling behavior of the susceptibilities and correlations between charges as shown in Fig. 4.

The pion sector is, however, different and has enhanced cutoff effects due to taste symmetry breaking. One does

not, therefore, expect to absorb all these effects with a choice of the temperature scale. For this reason we had to modify the HRG analysis to compare with lattice data for charge fluctuations which are dominated by contributions from the pions.

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- [1] H. Caines (STAR Collaboration), [arXiv:0906.0305](#); G. Odyniec (STAR Collaboration), *J. Phys. G* **35**, 104164 (2008).
 - [2] M. M. Aggarwal *et al.* (STAR Collaboration), *Phys. Rev. Lett.* **105**, 022302 (2010).
 - [3] M. Asakawa and K. Yazaki, *Nucl. Phys.* **A504**, 668 (1989).
 - [4] J. Berges and K. Rajagopal, *Nucl. Phys.* **B538**, 215 (1999); A. M. Halasz, A. D. Jackson, R. E. Shrock, M. A. Stephanov, and J. J. M. Verbaarschot, *Phys. Rev. D* **58**, 096007 (1998).
 - [5] F. Karsch, [arXiv:1202.4173](#).
 - [6] F. Karsch and K. Redlich, *Phys. Lett. B* **695**, 136 (2011).
 - [7] B. Friman, F. Karsch, K. Redlich, and V. Skokov, *Eur. Phys. J. C* **71**, 1694 (2011).
 - [8] P. Braun-Munzinger, B. Friman, F. Karsch, K. Redlich, and V. Skokov, *Phys. Rev. C* **84**, 064911 (2011).
 - [9] P. Braun-Munzinger, K. Redlich, and J. Stachel, in *Quark Gluon Plasma 3*, edited by R. C. Hwa and X.-N. Wang (World Scientific, Singapore, 2004), pp. 491–599.
 - [10] R. Dashen, S.-K. Ma, and H. J. Bernstein, *Phys. Rev.* **187**, 345 (1969).
 - [11] R. Venugopalan and M. Prakash, *Nucl. Phys.* **A546**, 718 (1992).
 - [12] F. Becattini, *J. Phys. Conf. Ser.* **5**, 175 (2005).
 - [13] J. Cleymans, H. Oeschler, K. Redlich, and S. Wheaton, *Phys. Rev. C* **73**, 034905 (2006).
 - [14] S. Ejiri, F. Karsch, and K. Redlich, *Phys. Lett. B* **633**, 275 (2006).
 - [15] A. Andronic, P. Braun-Munzinger, J. Stachel, and M. Winn, [arXiv:1201.0693](#).
 - [16] A. Andronic, P. Braun-Munzinger, and J. Stachel, *Phys. Lett. B* **673**, 142 (2009); **678**, 516(E) (2009).
 - [17] S. A. Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar, *Phys. Rev. Lett.* **59**, 2247 (1987).
 - [18] R. V. Gavai, S. Gupta, and P. Majumdar, *Phys. Rev. D* **65**, 054506 (2002).
 - [19] C. Bernard *et al.* (MILC Collaboration), *Phys. Rev. D* **71**, 034504 (2005).
 - [20] M. Cheng, P. Hegde, C. Jung, F. Karsch, O. Kaczmarek, E. Laermann, R. D. Mawhinney, C. Miao, P. Petreczky, C. Schmidt, and W. Soeldner, *Phys. Rev. D* **79**, 074505 (2009).
 - [21] S. Borsanyi, Z. Fodor, S. D. Katz, S. Krieg, C. Ratti, and K. Szabo, *J. High Energy Phys.* **01** (2012) 138.
 - [22] V. Koch, A. Majumder, and J. Randrup, *Phys. Rev. Lett.* **95**, 182301 (2005).
 - [23] C. R. Allton, M. Doring, S. Ejiri, S. J. Hands, O. Kaczmarek, F. Karsch, E. Laermann, and K. Redlich, *Phys. Rev. D* **71**, 054508 (2005).
 - [24] S. Mukherjee, *J. Phys. G* **38**, 124022 (2011).
 - [25] P. Hegde (HotQCD Collaboration), *AIP Conf. Proc.* **1441**, 898 (2012).
 - [26] E. Follana *et al.* (HPQCD Collaboration and UKQCD Collaboration), *Phys. Rev. D* **75**, 054502 (2007).
 - [27] A. Bazavov *et al.* (HotQCD Collaboration), *Phys. Rev. D* **85**, 054503 (2012).
 - [28] K. Nakamura *et al.* (Particle Data Group), *J. Phys. G* **37**, 075021 (2010).
 - [29] See for instance: J. Kapusta and C. Gale, *Finite Temperature Field Theory: Principles and Applications*, Cambridge Monographs on Mathematical Physics (Cambridge University Press, Cambridge, 2006).
 - [30] A. Bazavov *et al.* (MILC Collaboration), *Proc. Sci., LATTICE2010* (2010) 074.
 - [31] Y. Aoki, S. Borsanyi, S. Durr, Z. Fodor, S. D. Katz, S. Krieg, and K. K. Szabo, *J. High Energy Phys.* **06** (2009) 088.
 - [32] F. Karsch, K. Redlich, and A. Tawfik, *Phys. Lett. B* **571**, 67 (2003).
 - [33] P. Huovinen and P. Petreczky, *Nucl. Phys.* **A837**, 26 (2010).
 - [34] U. M. Heller, F. Karsch, and B. Sturmfels, *Phys. Rev. D* **60**, 114502 (1999).
 - [35] S. Jeon and V. Koch, *Phys. Rev. Lett.* **85**, 2076 (2000).
 - [36] A. Majumder and B. Muller, *Phys. Rev. C* **74**, 054901 (2006).
 - [37] J.-P. Blaizot, E. Iancu, and A. Rebhan, *Phys. Lett. B* **523**, 143 (2001).
 - [38] M. Kitazawa and M. Asakawa, *Phys. Rev. C* **85**, 021901 (2012).



Refining New-Physics Searches in $B \rightarrow D\tau\nu$ with Lattice QCD

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The semileptonic decay channel $B \rightarrow D\tau\nu$ is sensitive to the presence of a scalar current, such as that mediated by a charged-Higgs boson. Recently, the BABAR experiment reported the first observation of the exclusive semileptonic decay $B \rightarrow D\tau^- \bar{\nu}$, finding an approximately 2σ disagreement with the standard-model prediction for the ratio $R(D) = \text{BR}(B \rightarrow D\tau\nu)/\text{BR}(B \rightarrow D\ell\nu)$, where $\ell = e, \mu$. We compute this ratio of branching fractions using hadronic form factors computed in unquenched lattice QCD and obtain $R(D) = 0.316(12)(7)$, where the errors are statistical and total systematic, respectively. This result is the first standard-model calculation of $R(D)$ from *ab initio* full QCD. Its error is smaller than that of previous estimates, primarily due to the reduced uncertainty in the scalar form factor $f_0(q^2)$. Our determination of $R(D)$ is approximately 1σ higher than previous estimates and, thus, reduces the tension with experiment. We also compute $R(D)$ in models with electrically charged scalar exchange, such as the type-II two-Higgs-doublet model. Once again, our result is consistent with, but approximately 1σ higher than, previous estimates for phenomenologically relevant values of the scalar coupling in the type-II model. As a by-product of our calculation, we also present the standard-model prediction for the longitudinal-polarization ratio $P_L(D) = 0.325(4)(3)$.

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Motivation.—The third generation of quarks and leptons may be particularly sensitive to new physics associated with electroweak symmetry breaking due to their larger masses. For example, in the minimal supersymmetric extension of the standard model, charged-Higgs contributions to tauonic B decays can be enhanced if $\tan\beta$ is large. Thus, the semileptonic decay $B \rightarrow D\tau\nu$ is a promising new-physics search channel [1–13].

The BABAR experiment recently measured the ratios $R(D^{(*)}) = \text{BR}(B \rightarrow D^{(*)}\tau\nu)/\text{BR}(B \rightarrow D^{(*)}\ell\nu)$, where $\ell = e, \mu$, and reported excesses in both channels, which, when combined, disagree with the standard model by 3.4σ [14]. BABAR also interpreted these measurements

in terms of the type-II two-Higgs-doublet model (2HDM II) and claimed to exclude the theory at the 99.8% confidence level. In this Letter, we update the prediction for $R(D)$ in the standard model and in new-physics theories with a scalar current (such as the 2HDM II) using unquenched lattice-QCD calculations of the $B \rightarrow D\ell\nu$ form factors $f_0(q^2)$ and $f_+(q^2)$ by the Fermilab Lattice and MILC collaborations [15]. This is the first determination of $R(D)$ from *ab initio* full QCD.

With lepton helicity defined in the rest frame of the virtual W boson, the general expressions for the differential rates for semileptonic $B \rightarrow D\ell\nu$ decay are given by

$$\frac{d\Gamma_-}{dq^2} = \frac{1}{24\pi^3} \left(1 - \frac{m_\ell^2}{q^2}\right)^2 |p_D|^3 \times \left| G_V^{\ell cb} f_+(q^2) - \frac{m_\ell}{M_B} G_T^{\ell cb} f_2(q^2) \right|^2, \quad (1)$$

$$\begin{aligned} \frac{d\Gamma_+}{dq^2} = & \frac{1}{16\pi^3} \left(1 - \frac{m_\ell^2}{q^2}\right)^2 \frac{|p_D|}{q^2} \left\{ \frac{1}{3} |p_D|^2 \left| m_\ell G_V^{\ell cb} f_+(q^2) \right. \right. \\ & \left. \left. - \frac{q^2}{M_B} G_T^{\ell cb} f_2(q^2) \right|^2 + \frac{(M_B^2 - M_D^2)^2}{4M_B^2} \right. \\ & \left. \times \left| \left(m_\ell G_V^{\ell cb} - \frac{q^2}{m_b - m_c} G_S^{\ell cb} \right) f_0(q^2) \right|^2 \right\}, \quad (2) \end{aligned}$$

where the subscript denotes helicity and $q = (p_\ell + p_\nu)$ is the momentum carried by the charged lepton-neutrino pair. The total semileptonic width is the sum of the partial widths, $\Gamma_{\text{tot}} = (\Gamma_+ + \Gamma_-)$. At the tree level of the standard-model electroweak interaction, the scalar- and tensor-exchange couplings are $G_S = G_T = 0$, while the vector coupling is $G_V^{\ell ij} = G_F V_{ij}$. In the infinite heavy-quark-mass limit, the form factors $f_+(q^2)$ and $f_2(q^2)$ are related via

$$f_2(q^2) = -f_+(q^2) - \frac{M_B^2 - M_D^2}{q^2} [f_+(q^2) - f_0(q^2)]. \quad (3)$$

The form factor $f_2(q^2)$ is only relevant for theories with tensor currents, however, which we do not consider here.

Because the standard-model positive-helicity contribution to semileptonic $B \rightarrow D$ decay is proportional to the lepton mass squared, it can be neglected for the light leptons $\ell = e, \mu$; thus, experimental measurements of $B \rightarrow D\ell\nu$ decays are sensitive only to the vector form factor $f_+(q^2)$. On the other hand, the differential rate for $B \rightarrow D\tau\nu$ is sensitive also to the positive-helicity contribution and, hence, $f_0(q^2)$. Existing standard-model estimates of $d\Gamma_-/dq^2$ for $B \rightarrow D\tau\nu$ have relied on the kinematic constraint $f_0(0) = f_+(0)$, dispersive bounds on the shape [16], relations from heavy-quark symmetry, and quenched lattice QCD (neglecting u, d , and s quark loops) [17,18]. See Refs. [10–13] for details. In this Letter, we replace quenched QCD and heavy-quark estimates with a full, $2 + 1$ -flavor QCD calculation. In particular, we determine the following ratios within the standard model (where $\ell = e, \mu$):

$$R(D) = \text{BR}(B \rightarrow D\tau\nu) / \text{BR}(B \rightarrow D\ell\nu), \quad (4)$$

$$P_L(D) = (\Gamma_+^{B \rightarrow D\tau\nu} - \Gamma_-^{B \rightarrow D\tau\nu}) / \Gamma_{\text{tot}}^{B \rightarrow D\tau\nu}. \quad (5)$$

These quantities enable particularly clean tests of the standard model and probes of new physics because the Cabibbo-Kobayashi-Maskawa matrix elements and many of the hadronic uncertainties cancel between the numerator and denominator.

Lattice-QCD calculation.—Here, we briefly summarize the lattice-QCD calculation of the $B \rightarrow D\ell\nu$ semileptonic

form factors $f_+(q^2)$ and $f_0(q^2)$ [15]. Our calculation is based on a subset of the $2 + 1$ -flavor ensembles generated by the MILC Collaboration [19]. We use two lattice spacings, $a \approx 0.12$ and 0.09 fm, and two light-quark masses at each lattice spacing with (Goldstone) pion masses in the range 315–520 MeV; the specific numerical simulation parameters are given in Table I of Ref. [15].

This relatively small data set is sufficient for ratios such as those studied here and in Ref. [15], given the mild chiral and continuum extrapolations. We use the Fermilab action [20] for the heavy quarks (bottom and charm) and use the asqtad-improved staggered action [19] for the light valence and sea quarks (u, d, s). We minimize the systematic error due to contamination from radial excitations in two-point and three-point correlation functions by employing fits including their contributions, as described in Sec. III of Ref. [15]. We renormalize the lattice vector current $\bar{c}\gamma^\mu b$ (and other heavy-heavy currents) using a mostly nonperturbative method [21] in which we determine the flavor-conserving normalizations nonperturbatively. The remaining correction is close to unity and can be calculated in one-loop tadpole-improved lattice perturbation theory [22]. When extrapolating the lattice simulation results to the physical light-quark masses and the continuum limit, we carefully account for the leading nonanalytic dependence on the light-quark masses at nonzero but small momentum transfer [23], including the effects of lattice artifacts (generic discretization errors and taste-symmetry breaking introduced by the staggered action) [24,25]. The chiral-continuum extrapolation results are plotted in the left panels of Figs. 6 and 7 of Ref. [15]; for details, see Eqs. (4.1) and (4.2) of the same work and the surrounding text.

Figure 1 shows the results for $f_+(q^2)$ and $f_0(q^2)$ [15]. The simulated data are in the range $w < 1.17$ (to the left of the dashed vertical line), where $w = (M_B^2 + M_D^2 - q^2) / (2M_B M_D)$. In this region, we parametrize the w dependence of the form factors by a quadratic expansion of about $w = 1$, which works well for small recoil. To extend the form-factor results beyond the simulated recoil values (to the right of the dashed vertical line), we reparametrize the form factors in terms of the variable z [26] and then extrapolate to large recoil using a model-independent fit function based on general quantum theory principles of analyticity and crossing symmetry. The functional forms used to extrapolate $f_+(q^2)$ and $f_0(q^2)$ are defined in Eqs. (5.1)–(5.6) of Ref. [15]. The fits are plotted in the left panel of Fig. 9, and the results are given in the upper panel of Table V, both of the same work. As seen in Fig. 1, our result for $f_+(q^2)$ agrees very well with experimental measurements [27] over the full kinematic range. This nontrivial check gives confidence in the extrapolation of $f_0(q^2)$, which cannot be obtained experimentally and for which lattice-QCD input is crucial. In particular, lattice-QCD uncertainties are smallest near $q^2 = (M_B - M_D)^2$, so

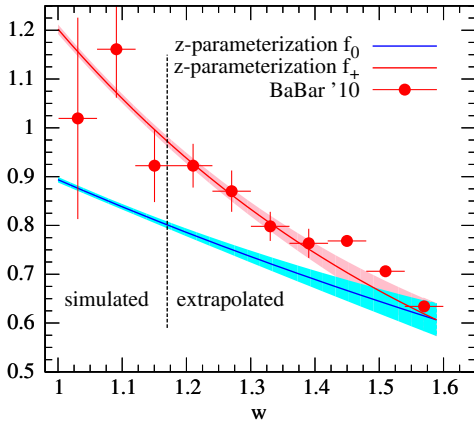


FIG. 1 (color online). The form factors f_+ [upper solid (red) line] and f_0 [lower solid (blue) line] from lattice QCD. The range of simulated recoil values is to the left of the vertical line. The filled colored bands show the interpolation or extrapolation of the numerical lattice data over the full kinematic range using the z parametrization. For comparison, the experimental measurement from *BABAR* [27] is shown as solid filled circles (using $|V_{cb}| = 41.4 \times 10^{-3}$ [17,27]).

the discussion below hinges principally on our calculation of $f_0(q^2)$ near this point, the validated $f_0(0) = f_+(0)$, and a smooth connection between the two limits.

We calculate the standard-model $B \rightarrow D\ell\nu$ partial decay rates into the three generations of leptons using these form factors and Eqs. (1) and (2) with $G_S = G_T = 0$, $G_V = G_F V_{cb}^*$. The resulting distributions are plotted in Fig. 2. To illustrate the role of the scalar form factor $f_0(q^2)$, we also show the rates with only the contributions from $f_+(q^2)$. Because of the significant helicity suppression, the differential decay rates into light leptons are well-approximated by a single contribution from the form factor $f_+(q^2)$. For $B \rightarrow D\tau\nu$, however, the contribution from the scalar form factor $f_0(q^2)$ comprises half of the standard-model rate.

Given the lattice-QCD determinations of $f_+(q^2)$ and $f_0(q^2)$, we can obtain the standard-model values for $R(D)$ and $P_L(D)$. These are the primary results of this Letter, and we now discuss the sources of systematic uncertainty. In Ref. [15], many statistical and several systematic errors cancelled approximately or exactly in the ratio $f_0^{B \rightarrow D_s \ell \nu} / f_0^{B \rightarrow D \ell \nu}$ studied there. Some of these do not cancel (as well) in $R(D)$ and $P_L(D)$, however, because they affect $f_+(q^2)$ and $f_0(q^2)$ differently.

Table I shows the error budgets for $R(D)$ and $P_L(D)$. The statistical error in $R(D)$ is significant (3.7%) due to the different phase-space integrations in the numerator and denominator, whereas for $P_L(D)$ the correlated statistical fluctuations largely cancel. For the same reason, the errors in $R(D)$ arising from the extrapolation to the physical light-quark masses and the continuum limit (1.4%) and to the full q^2 range (1.5%) are much larger than for $P_L(D)$. We estimate the error from the chiral-continuum extrapolation

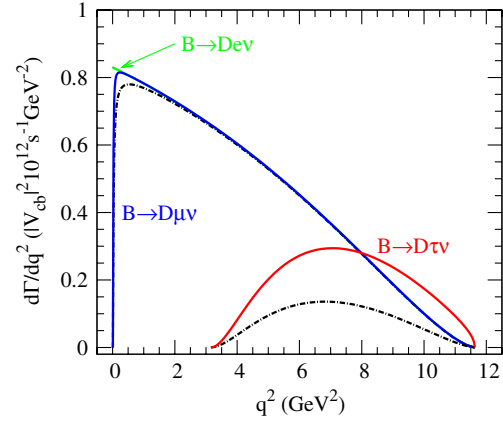


FIG. 2 (color online). Differential decay rates in the standard model for $B \rightarrow D\ell\nu$, $B \rightarrow D\mu\nu$, and $B \rightarrow D\tau\nu$ (solid lines, as labeled). The black dash-dotted curves show the rates calculated with $f_0(q^2) = 0$.

by comparing the results for fits with and without next-to-next-to-leading-order analytic terms in the chiral expansion. We estimate the error from the z extrapolation by varying the range of synthetic data used in the z fit, including an additional pole in the fit function and including higher powers of z . The specific chiral and z -fit variations considered are enumerated in Table VI of Ref. [15] and discussed in detail in the surrounding text. The remaining sources of uncertainty in Table I do not contribute significantly to the quantities studied in Ref. [15], so we describe them in greater detail below.

We determine the bare heavy-quark masses in our simulations by tuning the parameters κ_b and κ_c in the heavy-quark action such that the kinetic masses of the pseudoscalar B_s and D_s mesons match the experimentally measured values [20]. In practice, it is easier to work with the form factors $h_{\pm}(w)$ on the lattice, which are linear combinations of $f_{+,0}(q^2)$ [15]. We study how the form factors $h_{\pm}(w)$ depend on $\kappa_{b,c}$ by recomputing the form factors on some ensembles at values of $\kappa_{b,c}$ slightly above and below the default ones and extracting the slopes with respect to $\kappa_{b,c}$. We use these slopes to correct our results for $R(D)$ and $P_L(D)$ slightly from the simulated κ values to

TABLE I. Error budgets for the branching-fraction and longitudinal-polarization ratios discussed in the text. Errors are given as percentages.

Source	$R(D)$	$P_L(D)$
Monte Carlo statistics	3.7	1.2
Chiral-continuum extrapolation	1.4	0.1
z expansion	1.5	0.1
Heavy-quark-mass (κ) tuning	0.7	0.1
Heavy-quark discretization	0.2	0.3
Current $\rho_{V_{cb}^{i_1}} / \rho_{V_{cb}^0}$	0.4	0.7
Total	4.3%	1.5%

the physical ones, and conservatively take the full size of the shift as the error due to κ tuning.

We remove the leading taste-breaking light-quark discretization errors in the form factors with the chiral-continuum extrapolation and estimate the remaining discretization errors from the heavy-quark action with power counting [28]. We compute both the coefficient of the dimension 5 operator in the Fermilab action c_{SW} and the rotation parameter d_1 for the heavy-quark fields at the tree level in tadpole-improved lattice perturbation theory [20]. Then, the leading heavy-quark errors in $h_+(1)$ are of $O[\alpha_s(\Lambda/2m_Q)^2]$ and $O[(\Lambda/2m_Q)^3]$, where Λ is a typical hadronic scale. Using the values $\alpha_s = 0.3$, $\Lambda = 500$ MeV, and $m_c = 1.2$ GeV, we estimate that heavy-quark discretization errors in $h_+(1)$ are ~ 1 – 2% . At nonzero recoil, $w > 1$, there are corrections to $h_+(w)$ of $O(\alpha_s \Lambda/2m_Q)$, but these are suppressed by $(1 - w)$ because they vanish in the limit $w = 1$ by Luke's theorem [29]. We expect them to be largest at our highest recoil point $w = 1.2$ and estimate their size to be $\sim 1\%$. Thus, we estimate the uncertainty in $h_+(w)$ from heavy-quark discretization errors to be 2% , which leads to negligible errors in $R(D)$ and $P_L(D)$. The leading heavy-quark error in $h_-(w)$ is of $O(\alpha_s \Lambda/2m_Q)$, which we estimate with the input parameters above to be $\sim 6\%$. To be conservative, we take the error in the ratio $h_-(w)/h_+(w)$ to be 10% , which leads to small errors in $R(D)$ and $P_L(D)$.

Our methods for computing $B \rightarrow D$ transitions incorporate the bulk of the matching of the lattice vector current to continuum automatically, leaving a factor $\rho_{V_{cb}^\mu}$ close to unity [30]. For $R(D)$ and $P_L(D)$, only the relative matching of the spatial and temporal components of the current matters, $\rho_{V_{cb}^i}/\rho_{V_{cb}^0}$. Although we have a one-loop calculation of $\rho_{V_{cb}^0}$ in hand, no nontrivial result for $\rho_{V_{cb}^i}$ is available. We take $\rho_{V_{cb}^i}/\rho_{V_{cb}^0} = 1.0 \pm 0.2$ to estimate the uncertainty from this source. In similar calculations, we have never seen ρ factors that differ from unity by more than 5% , so this range is extremely conservative. The uncertainty in the current renormalization factors leads to a small error in $R(D)$ but is the second-largest source of error in $P_L(D)$, after statistics.

We also consider the systematic uncertainties from tuning the light-quark masses and determining the absolute lattice scale r_1 , but these produce negligible errors in both $R(D)$ and $P_L(D)$.

Results and conclusions.—We obtain the following determinations for the branching-fraction and longitudinal-polarization ratios for $B \rightarrow D \ell \nu$ semileptonic decay:

$$R(D) = 0.316(12)(7), \quad (6)$$

$$P_L(D) = 0.325(4)(3), \quad (7)$$

where the errors are statistical and total systematic, respectively. The value of $R(D)$ is approximately 1σ larger than the recent standard-model values obtained using estimates

of $f_0(q^2)$ from Refs. [11,13] but it is still 1.7σ lower than the recent *BABAR* measurement, $R(D) = 0.440 \pm 0.058 \pm 0.042$ [14]. The results for $R(D)$ from Belle [31] agree with those of *BABAR* but have larger uncertainties. Current experimental measurements of $R(D)$ are statistics-limited, so the luminosities available at Belle II and SuperB should enable significant improvement on $R(D)$ and possibly a determination of $P_L(D)$.

We also reexamine the interpretation of the *BABAR* measurement of $R(D)$ as a constraint on the 2HDM II; the result is plotted in Fig. 3. For this theory, the scalar-exchange coupling in Eq. (2) is given by

$$G_S^{\ell cb} = G_F V_{cb} \frac{m_\ell(m_c + m_b \tan^2 \beta)}{M_{H^\pm}^2}. \quad (8)$$

As soon as $\tan \beta \gtrsim 4$, m_c in Eq. (8) can be neglected. On the other hand, evaluating Eq. (2) depends sensitively on m_c/m_b via the prefactor multiplying $f_0(q^2)$. We take $m_c/m_b = 0.22$, following Refs. [13,14]. Our improved calculation of the scalar form factor $f_0(q^2)$ increases the prediction for $R(D)$ by about 1σ for all $\tan \beta/M_{H^\pm} < 0.6 \text{ GeV}^{-1}$. This sensitivity of $R(D)$ to differences in $f_0(q^2)$ suggests that one should be cautious in using indirect estimates of the form factors to constrain new-physics models in other decay channels such as $B \rightarrow D^* \tau \nu$.

Inspection of the general formulas for the differential decay rates, Eqs. (1) and (2), shows that many new-physics explanations for the $\sim 3\sigma$ tension between measurements of $\{R(D), R(D^*)\}$ and the standard model are possible. Even in the context of 2HDM, variants other than type II can have different phenomenologies [32]. Lattice-QCD calculations of $f_+(q^2)$ and $f_0(q^2)$ can be used to provide reliable predictions for $R(D)$ in any model, given values for the

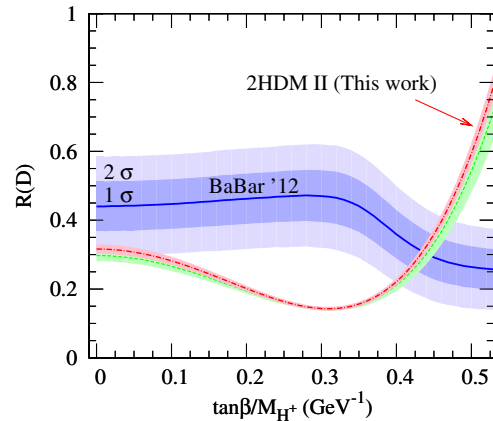


FIG. 3 (color online). Lattice-QCD calculation [dash-dotted (red) line] and experimental measurement [14] [solid (blue) line] of $R(D)$ vs $\tan \beta/M_{H^\pm}$ in the 2HDM II. For the *BABAR* result, the dark (light) blue regions denote the 1σ (2σ) error bands. For comparison, the 2HDM II curve based on Refs. [11,13] and used in Ref. [14] is shown as a dashed green line.

couplings $\{G_S, G_V, G_T\}$. We note, however, that the Dalitz distribution for the lepton and D -meson energies in the B -meson rest frame may be more sensitive to tensor interactions than $R(D)$ [33].

The largest source of uncertainty in our determinations of $R(D)$ and $P_L(D)$ is statistical errors, which we expect to reduce with an analysis of our full data set in a future work [34]. The ratio $R(D)$ is correlated with $P_L(D)$, as well as other observables such as $R(D^*)$ or $R(D_s)$ in many new-physics models; thus, the pattern of experimental results for these quantities can help distinguish between new-physics scenarios, such as those with and without a charged-Higgs boson [12]. We will present lattice-QCD results for $R(D^*)$ and $P_L(D^*)$ in a future paper on the $B \rightarrow D^* \ell \nu$ form factors, and also note that we could easily obtain standard-model predictions for $R(D_s)$ and $P_L(D_s)$ if measurements of these quantities were possible with an $Y(5S)$ run at a B factory.

Given the present tensions between experimental measurements and standard-model predictions for both $\{R(D), R(D^*)\}$ and the leptonic branching fraction $\text{BR}(B \rightarrow \tau \nu)$ [35–38], lattice-QCD calculations of $B \rightarrow D \tau \nu$ form factors and other hadronic weak matrix elements can play a key role in revealing whatever theory beyond the standard model is realized in nature.

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- [1] B. Grzadkowski and W.-S. Hou, *Phys. Lett. B* **283**, 427 (1992).
- [2] M. Tanaka, *Z. Phys. C* **67**, 321 (1995).
- [3] R. Garisto, *Phys. Rev. D* **51**, 1107 (1995).
- [4] Y. S. Tsai, *Nucl. Phys. B, Proc. Suppl.* **55**, 293 (1997).
- [5] G.-H. Wu, K. Kiers, and J. N. Ng, *Phys. Rev. D* **56**, 5413 (1997).
- [6] K. Kiers and A. Soni, *Phys. Rev. D* **56**, 5786 (1997).
- [7] T. Miki, T. Miura, and M. Tanaka, *arXiv:hep-ph/0210051*.
- [8] H. Itoh, S. Komine, and Y. Okada, *Prog. Theor. Phys.* **114**, 179 (2005).
- [9] C.-H. Chen and C.-Q. Geng, *J. High Energy Phys.* **10** (2006) 053.
- [10] U. Nierste, S. Trine, and S. Westhoff, *Phys. Rev. D* **78**, 015006 (2008).
- [11] J. F. Kamenik and F. Mescia, *Phys. Rev. D* **78**, 014003 (2008).
- [12] M. Tanaka and R. Watanabe, *Phys. Rev. D* **82**, 034027 (2010).
- [13] S. Fajfer, J. F. Kamenik, and I. Nisandzic, *Phys. Rev. D* **85**, 094025 (2012).
- [14] J. P. Lees *et al.* (BABAR Collaboration), *arXiv:1205.5442*.
- [15] J. A. Bailey *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **85**, 114502 (2012).
- [16] I. Caprini, L. Lellouch, and M. Neubert, *Nucl. Phys.* **B530**, 153 (1998).
- [17] G. de Divitiis, E. Molinaro, R. Petronzio, and N. Tantalo, *Phys. Lett. B* **655**, 45 (2007).
- [18] G. de Divitiis, R. Petronzio, and N. Tantalo, *J. High Energy Phys.* **10** (2007) 062.
- [19] A. Bazavov *et al.*, *Rev. Mod. Phys.* **82**, 1349 (2010).
- [20] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, *Phys. Rev. D* **55**, 3933 (1997).
- [21] A. X. El-Khadra, A. S. Kronfeld, P. B. Mackenzie, S. M. Ryan, and J. N. Simone, *Phys. Rev. D* **64**, 014502 (2001).
- [22] G. P. Lepage and P. B. Mackenzie, *Phys. Rev. D* **48**, 2250 (1993).
- [23] C.-K. Chow and M. B. Wise, *Phys. Rev. D* **48**, 5202 (1993).
- [24] C. Aubin and C. Bernard, *Phys. Rev. D* **73**, 014515 (2006).
- [25] J. Laiho and R. S. Van de Water, *Phys. Rev. D* **73**, 054501 (2006).
- [26] C. G. Boyd, B. Grinstein, and R. F. Lebed, *Phys. Rev. D* **56**, 6895 (1997).
- [27] B. Aubert *et al.* (BABAR Collaboration), *Phys. Rev. Lett.* **104**, 011802 (2010).

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- [28] A. S. Kronfeld, [Phys. Rev. D **62**, 014505 \(2000\)](#).
[29] M. E. Luke, [Phys. Lett. B **252**, 447 \(1990\)](#).
[30] J. Harada, S. Hashimoto, A. S. Kronfeld, and T. Onogi, [Phys. Rev. D **65**, 094514 \(2002\)](#).
[31] I. Adachi *et al.* (Belle Collaboration), [arXiv:0910.4301](#).
[32] A. Crivellin, C. Greub, and A. Kokulu, [arXiv:1206.2634](#).
[33] A. S. Kronfeld, Proc. Sci., LATTICE2008 (2008) 282 [[arXiv:0812.2030](#)].
[34] S.-W. Qiu *et al.* (Fermilab Lattice and MILC Collaborations), Proc. Sci., LATTICE2011 (2011) 289 [[arXiv:1111.0677](#)].
[35] M. Bona *et al.* (UTfit Collaboration), [Phys. Lett. B **687**, 61 \(2010\)](#).
[36] E. Lunghi and A. Soni, [Phys. Lett. B **697**, 323 \(2011\)](#).
[37] J. Charles *et al.*, [Phys. Rev. D **84**, 033005 \(2011\)](#).
[38] J. Laiho, E. Lunghi, and R. Van de Water, Proc. Sci., LATTICE2011 (2011) 018 [[arXiv:1204.0791](#)].

Charm and bottom heavy baryon mass spectrum from lattice QCD with 2+1 flavors

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We present results for the mass spectrum of charm and bottom heavy baryons, using MILC coarse lattice configurations with 2+1 flavors. Clover heavy quark propagators with the Fermilab interpretation and improved staggered light quark propagators are used to construct two point functions with local operators for different flavor and spin states.

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1. Introduction

Heavy baryons have been extensively investigated by experimental and theoretical approaches. From experiment, the singly charmed heavy baryon mass spectrum is well known; however, the other heavy baryon masses are only crudely known. Recently, from the $D0$ [1] and CDF [2] collaborations, there are measurements of the mass of the singly bottom baryon Ξ_b^- . From lattice QCD, there are several quenched calculations for the heavy baryon mass spectrum [3–8], and most results are in fair agreement with observed values. In this project, we apply lattice QCD with dynamical sea quarks for the same objective.

Previously, we have presented the preliminary results for the mass spectrum of singly charmed heavy baryons [9]. Here, we present the singly charmed and bottom heavy baryon as well as the doubly charmed and bottom heavy baryon mass spectrum. In this work, we use two different interpolating operators studied in Ref. [3], and construct two-point functions using the method of Wingate *et al.* [10] to combine staggered propagators for the light valence quarks and a Wilson type (clover) propagator for the heavy valence quark. In addition, we show that there is no taste mixing problem by studying the explicit spin and taste structure of operators.

2. Construction of two-point functions

The interpolating operators to describe singly heavy baryons are [3]

$$\mathcal{O}_5 = \varepsilon_{abc}(\psi_1^{aT} C \gamma_5 \psi_2^b) \Psi_H^c, \quad \mathcal{O}_\mu = \varepsilon_{abc}(\psi_1^{aT} C \gamma_\mu \psi_2^b) \Psi_H^c, \quad (2.1)$$

where ε_{abc} is the Levi-Civita tensor, ψ_1 and ψ_2 are light valence quark fields for up, down, or strange quarks, Ψ_H is the heavy valence quark field for the charm or the bottom quark, C is the charge conjugation matrix, and a , b , and c are color indices. Basically, $\mathcal{O}_5$ is the operator for $s^\pi = 0^+$, and $\mathcal{O}_\mu$ is for $s^\pi = 1^+$, where s^π is the spin parity state for the light quark pair. As can be seen, the spinor indices of the light quark fields are contracted together, so the spinor index of the operator comes from Ψ_H . Furthermore, each heavy baryon is obtained by choosing appropriate quark flavor combinations, and, for doubly heavy baryons, we can simply interchange the heavy quark field and the light quark fields in Eq. 2.1 [4].

Since we use staggered fermion propagators for the light quarks, and a Wilson type propagator for the heavy quark, we will use the method of Wingate *et al.* [10] to convert to a naive quark propagator starting from a staggered propagator. They show

$$G_\psi(x, y) = \Omega(x) \Omega^\dagger(y) G_\chi(x, y), \quad (2.2)$$

where

$$\Omega(x) = \prod_\mu (\gamma_\mu)^{x_\mu/a}, \quad (2.3)$$

$G_\psi(x, y)$ is the naive quark propagator, and $G_\chi(x, y)$ is the staggered quark propagator. With this basic relationship, we can construct the heavy baryon two-point functions for $s^\pi = 0^+$ using the operator $\mathcal{O}_5$.

$$C_5(\vec{p}, t) = \sum_{\vec{x}} e^{-i\vec{p} \cdot \vec{x}} \langle \mathcal{O}_5(\vec{x}, t) \overline{\mathcal{O}}_5(\vec{0}, 0) \rangle \quad (2.4)$$

$$= \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \epsilon_{abc} \epsilon_{a'b'c'} \text{tr}[G_1^{aa'T}(x,0) C \gamma_5 G_2^{bb'}(x,0) C \gamma_5] G_H^{cc'}(x,0) \quad (2.5)$$

$$= \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \epsilon_{abc} \epsilon_{a'b'c'} 4 G_{1\chi}^{aa'}(x,0) G_{2\chi}^{bb'}(x,0) G_H^{cc'}(x,0). \quad (2.6)$$

$G_1(x,0)$ and $G_2(x,0)$ are naive light quark propagators, $G_H(x,0)$ is the Wilson type heavy quark propagator, and $G_{1\chi}(x,0)$ and $G_{2\chi}(x,0)$ are staggered light quark propagators. Note that the trace in Eq. 2.5 is for spinor indices, not for color indices. Similarly, we can derive the two-point function for $s^\pi = 1^+$ with the operator $\mathcal{O}_\mu$, which is

$$C_{\mu\nu}(\vec{p},t) = \sum_{\vec{x}} e^{-i\vec{p}\cdot\vec{x}} \epsilon_{abc} \epsilon_{a'b'c'} 4(-1)^{x_\mu} \delta_{\mu\nu} G_{1\chi}^{aa'}(x,0) G_{2\chi}^{bb'}(x,0) G_H^{cc'}(x,0). \quad (2.7)$$

We note that $\delta_{\mu\nu}$ in Eq. 2.7 is an artifact of using Eq. 2.2 to convert the light staggered propagator to a naive propagator. With Wilson or clover light quarks, $C_{\mu\nu}$ would have off diagonal elements. We shall now elucidate the origin of the δ -function.

3. Taste mixing

We know that heavy-light mesons do not have any taste mixing problem [10]. Since we use two staggered quarks for singly heavy baryons, the taste structure of the operators might be more complicated than in the heavy-light meson case. Furthermore, presence of the δ function in Eq. 2.7 suggests we investigate more seriously.

We have resolved this problem by considering the taste and spin structure of the operators explicitly. Let's look at the operator $\mathcal{O}_\mu$ in Eq. 2.1. Since the heavy quark field Ψ_H carries no taste index, we can simplify the problem by considering the di-quark operator $\mathcal{D}_\mu$ rather than the original operator $\mathcal{O}_\mu$, i.e.,

$$\mathcal{D}_\mu = \psi_1^T C \gamma_\mu \psi_2. \quad (3.1)$$

Next, we have a relation between the naive quark and the staggered quark fields

$$\psi^{\alpha'}(x) = \Omega^{\alpha'a}(x) \chi^a(x), \quad (3.2)$$

where $\psi^{\alpha'}$ is the naive quark, χ^a are four copies of staggered quark, $\Omega(x)$ is the matrix given in Eq. 2.3, α' is the spinor index of the naive quark, and a is the copy index. Also, we have

$$\chi^a(y+\xi) = 2\Omega^{\dagger i\alpha}(\xi) q^{\alpha i,a}(y) \quad (3.3)$$

and

$$x = y + \xi, \quad (3.4)$$

where $q^{\alpha i,a}$ is the staggered quark in the taste basis, α is the staggered spin index, i is the taste index, x is the coordinate index for all lattice sites, y is the coordinate index for even sites only, and ξ is the vector of each corner of the unit hypercube. Using Eqs. 3.2 and 3.3, we can rewrite the naive quark $\psi^{\alpha'}(x)$ as a linear combination of the staggered quarks in the taste basis

$$\psi^{\alpha'}(x) = \Omega^{\alpha'a}(\xi) \chi^a(y+\xi) = \Omega^{\alpha'a} 2\Omega^{\dagger i\alpha}(\xi) q^{\alpha i,a}(y). \quad (3.5)$$

Now, we can put Eq. 3.5 into the di-quark operator, and sum over the hypercube in order to get the continuum di-quark operator $\mathcal{D}_\mu^{conti}(y)$,

$$\begin{aligned}\mathcal{D}_\mu^{conti}(y) &= \sum_{\xi} (\psi_1^T(x) C \gamma_\mu \psi_2(x)) \\ &= \sum_{\xi} 2\Omega^{\dagger i\alpha}(\xi) q^{\alpha i, a}(y) \Omega^{Ta\alpha'}(\xi) (C \gamma_\mu)^{\alpha' \beta'} \Omega^{\beta' b}(\xi) 2\Omega^{\dagger j\beta}(\xi) q^{\beta j, b}(y) \\ &= \sum_{\xi} 4\Omega^{\dagger i\alpha}(\xi) q^{\alpha i, a}(y) (-1)^{\xi_\mu} (C \gamma_\mu)^{ab} \Omega^{\dagger j\beta}(\xi) q^{\beta j, b}(y),\end{aligned}\quad (3.6)$$

using the relation

$$\Omega^{Ta\alpha'}(\xi) (C \gamma_\mu)^{\alpha' \beta'} \Omega^{\beta' b}(\xi) = (-1)^{\xi_\mu} (C \gamma_\mu)^{ab}. \quad (3.7)$$

Next we sum over ξ in Eq. 3.6, using

$$\sum_{\xi} \Omega^{\dagger i\alpha}(\xi) (-1)^{\xi_\mu} \Omega^{\dagger j\beta}(\xi) = 4(C \gamma_\mu)^{\alpha\beta} \otimes (\gamma_\mu C^{-1})^{ij}. \quad (3.8)$$

Finally, the continuum di-quark operator $\mathcal{D}_\mu^{conti}(y)$ can be written

$$\mathcal{D}_\mu^{conti}(y) = 16q^{\alpha i, a}(y) (C \gamma_\mu)^{\alpha\beta} \otimes (\gamma_\mu C^{-1})^{ij} q^{\beta j, b}(y) (C \gamma_\mu)^{ab}. \quad (3.9)$$

From Ref. [11], we immediately notice that this continuum di-quark operator $\mathcal{D}_\mu^{conti}$ overlaps with a physical $s^\pi = 1^+$ spin parity state with a taste singlet. Thus, the original operator $\mathcal{O}_\mu$ overlaps with $\frac{1}{2}^+$ and $\frac{3}{2}^+$ total spin parity states of the heavy baryon without any taste mixing problem in the continuum limit.

Similarly, we can easily derive the continuum di-quark operator $\mathcal{D}_5^{conti}$ for the operator $\mathcal{O}_5$

$$\mathcal{D}_5^{conti}(y) = 16q^{\alpha i, a}(y) (C \gamma_5)^{\alpha\beta} \otimes (\gamma_5 C^{-1})^{ij} q^{\beta j, b}(y) (C \gamma_5)^{ab}, \quad (3.10)$$

and we can state that the operator $\mathcal{O}_5$ overlaps with physical $\frac{1}{2}^+$ total spin parity state of the singly heavy baryon with a taste singlet for the same reason.

In addition, if we consider the two-point function $C_{\mu\nu}^{conti}$ of the continuum di-quark operator $\mathcal{D}_\mu^{conti}$, then it appears

$$\begin{aligned}C_{\mu\nu}^{conti}(y; 0) &= 16^2 \text{Tr}[G_1(y, 0) (C \gamma_\mu) \otimes (C \gamma_\mu)^\dagger G_2(y, 0) (C \gamma_\nu)^\dagger \otimes (C \gamma_\nu)] \\ &\quad \times (C \gamma_\mu)_{ab} (\gamma_\nu C^{-1})_{b'a'} \delta_{bb'} \delta_{aa'}\end{aligned}\quad (3.11)$$

$$\begin{aligned}&= 16^2 \text{Tr}[G_1(y, 0) (C \gamma_\mu) \otimes (C \gamma_\mu)^\dagger G_2(y, 0) (C \gamma_\nu)^\dagger \otimes (C \gamma_\nu)] \\ &\quad \times \text{Tr}[(C \gamma_\mu) (C \gamma_\nu)^\dagger],\end{aligned}\quad (3.12)$$

where

$$\text{Tr}[(C \gamma_\mu) (C \gamma_\nu)^\dagger] = 4\delta_{\mu\nu}. \quad (3.13)$$

As we can see from Eq. 3.12, $C_{\mu\nu}^{conti}(y; 0)$ consists of two traces. The first trace contains spinor and taste indices. The second trace is over copy indices. Now, we can address where the delta function in Eq. 2.7 came from: cancellations of the copy indices govern the delta function. Furthermore, we notice that even though the copy indices have a non-trivial structure, we can still use the operator $\mathcal{O}_\mu$, because the contribution of the copy indices is a constant, and independent of spin and taste.

4. Results

We use three ensembles of $20^3 \times 64$ MILC coarse dynamical lattice gauge configurations with lattice spacing $a \approx 0.12$ fm [12]. The details of the ensembles are shown in Table 1. For each configuration, we require several propagators for the valence quarks. We compute nine different staggered light quark propagators with masses between 0.005 and 0.02, and three staggered strange quark propagators with masses 0.024, 0.03, and 0.0415, and each propagator is calculated with four different time sources. For the heavy quarks, we use hopping parameter values $\kappa = 0.122$ for the charm quark, and $\kappa = 0.086$ for the bottom quark based on tuning for our heavy-light meson decay constant calculation [13] [14].

β	am_l	am_s	# of conf. for charm	# of conf. for bottom
6.76	0.007	0.05	545	554
6.76	0.01	0.05	591	590
6.79	0.02	0.05	459	452

Table 1: Parameters of the ensembles, and number of configurations used for each heavy quark. The light sea quark mass is m_l and the strange sea quark mass is m_s .

For the data analysis for the baryon propagators, we use the same fitting and extrapolation method as in our previous work [9].

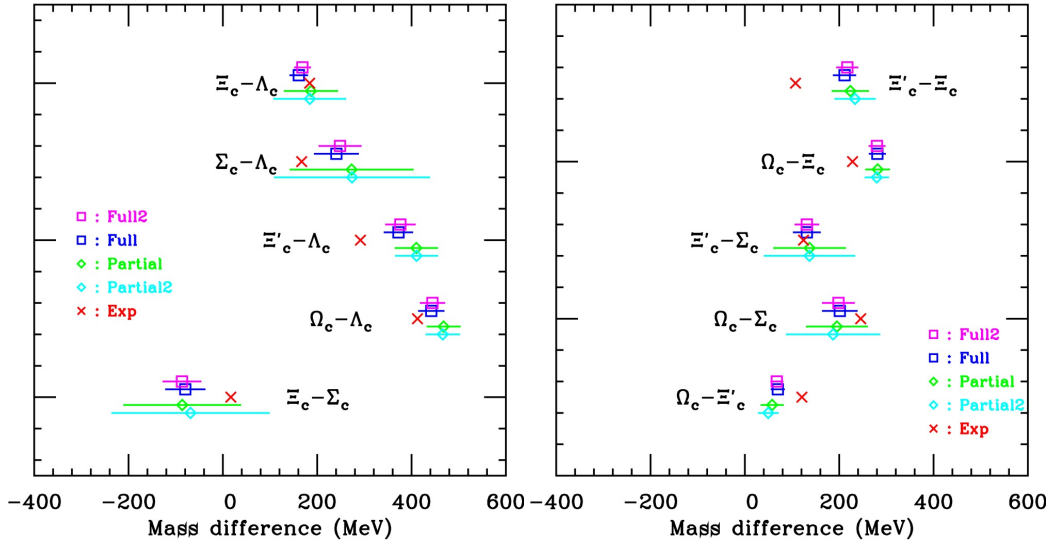


Figure 1: The mass splittings for singly charmed heavy baryons.

We present mass splittings in MeV for singly charmed heavy baryons in Fig. 1. Crosses correspond to the experimental data [15], and squares and diamonds with error bars indicate our results. The experimental errors are considerably smaller than our own, so we ignore them here, and the errors of our results are statistical errors. Since we do not have partially quenched staggered chiral perturbation theory for singly heavy baryons to fit both sea and valence quark mass dependences simultaneously, we use four slightly different extrapolation methods. The result from each method

is labeled as Full, Full2, Partial, or Partial2 in Fig. 1. The first method takes all partially quenched data, and linearly extrapolates for the valence quark masses and then the sea quark masses; this is the “Partial” result. Alternatively, we consider only data where light valence masses equal the corresponding sea quark mass and do a single extrapolation; this is the “Full” data. Further, we can obtain the mass splittings by a second method. Instead of applying the chiral extrapolations to the masses themselves, we apply them to the splittings. Results from the second procedure are denoted with a “2”.

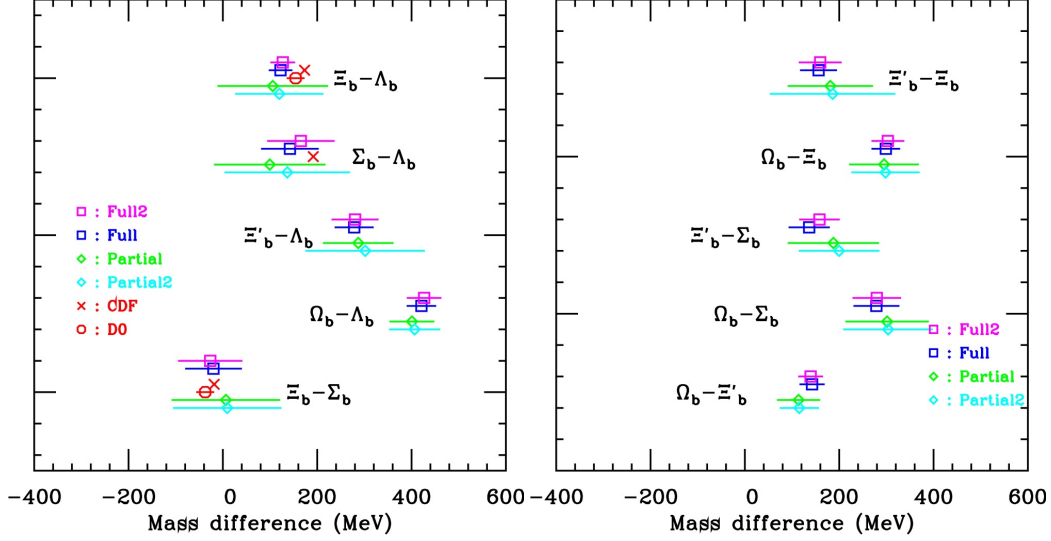


Figure 2: The mass splittings for singly bottom heavy baryons.

We also present mass splittings for singly bottom heavy baryons in Fig. 2. Crosses are the recent experimental data from the CDF [2], and octagons are the experiment data from the D0 [1]. We include error bars for the D0 results, since the errors of the D0 results are larger than the other experiments, about 18 MeV.

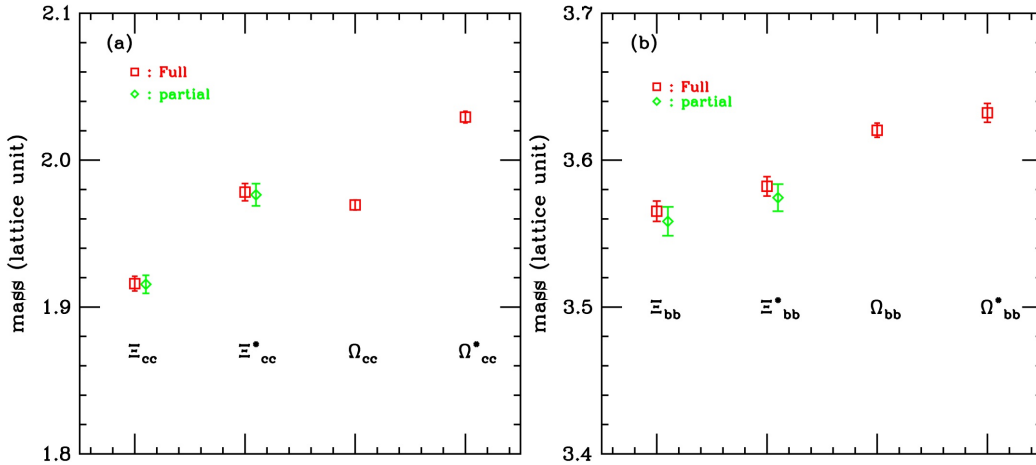


Figure 3: The mass spectrum for doubly charm (a), and bottom (b) heavy baryons.

In addition, we present a preliminary mass spectrum in lattice units for doubly bottom and

charmed heavy baryons in Fig. 3.

5. Future study

We have presented the mass spectrum for charm and bottom heavy baryons based on dynamical lattice QCD, and a solution of the taste mixing problem of the operators. The study can be extended in several ways. In the near future, we would like to extend this work into $28^3 \times 96$ MILC fine lattice gauge configurations; so that we can determine the mass spectrum more accurately. In this work, we apply the simple linear extrapolations for sea quark masses and valence quark masses separately; as a result, our partially quenched data analysis gives larger errors than the errors from full QCD data analysis. In order to extrapolate for the both sea and valence quark masses simultaneously and accurately, we would like to develop partially quenched staggered chiral perturbation theory for heavy baryons. Next, we must consider systematic errors, such as finite size effects and discretization errors. In addition, we are interested in the $\frac{3}{2}^+$ excited state masses of singly heavy baryons, which cannot be studied with our current method.

Acknowledgments

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References

- [1] A.M. Abazov *et al.*, Phys. Rev. Lett. **99** (2007) 052001.
- [2] T. Aaltonen *et al.*, Phys. Rev. Lett. **99** (2007) 052002.
- [3] K.C. Bowler *et al.* (UKQCD Collaboration), Phys. Rev. D **54** (1996) 3619.
- [4] N. Mathur *et al.*, Phys. Rev. D **66** (2002) 014502.
- [5] R.M. Woloshyn, Phys. Lett. B **476** (2000) 309.
- [6] S. Gottlieb and S. Tamhankar, Nucl. Phys. Proc. Suppl. **119** (2003) 644.
- [7] A. Ali Khan *et al.*, Phys. Rev. D **62** (2000) 054505.
- [8] T.W. Chiu and T.H. Hsieh, Nucl. Phys. A **755** (2005) 471c.
- [9] H. Na and S. Gottlieb, PoS (LAT2006) 191 [hep-lat/0610009].
- [10] M. Wingate *et al.*, Phys. Rev. D **67** (2003) 054505.
- [11] S. Gottlieb, H. Na, and K. Nagata, arXiv:0707.3537 [hep-lat].
- [12] C. W. Bernard *et al.*, Phys. Rev. D **64**, 054506 (2001) [hep-lat/0104002].
- [13] C. Aubin *et al.* (Fermilab Lattice, MILC, and HPQCD Collaborations), Phys. Rev. Lett. **95** (2005) 122002.
- [14] C. Aubin *et al.* (Fermilab Lattice, MILC, and HPQCD Collaborations), Phys. Rev. Lett. **94** (2005) 011601.
- [15] W.M. Yao *et al.*, J. Phys. G **33** (2006) 1.

Sharing lattices throughout the world: an ILDG status report

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The international lattice data grid, a system for sharing gauge configuration files throughout the world, is operational for the most part. I give a status report, give some pointers on accessing lattice files, and highlight some of the available gauge configurations.

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1. Introduction

The rapid expansion of internet services in the 1990's made it easy to publish gauge configuration files for general public access. The US Gauge Connection at NERSC was established in 1997 for this purpose[1]. It was simple and effective, but it was not the ideal solution for broad international use. The development of a truly international lattice data grid (ILDG) began some years later (2002) as a result of discussions organized by the UKQCD [2]. Its primary purpose is to facilitate the advancement of our field by making it easy for scientific collaborations to share gauge configuration files with other collaborations throughout the world. To reach this goal required first the development of regional or national grids for intraregional file sharing and storage. This effort typically exploited existing grid infrastructure and tools. The ILDG was then built upon the regional grids.

As a consequence of this history, the ILDG is a consortium of autonomous regional grids [3]. Current participants are centered in Australia (CSSM), Europe (Austria, Switzerland, Germany, France, Italy)(LDG), Japan (JLDG), the United Kingdom (QCDGrid or DiGS), and the United States. Additional participants are, of course, always welcome. Cooperation involves the standardization of several components: binary file formats, metadata markup schema (QCDml), user authentication methods, and replica-catalog and file-transfer interoperability. These standards are achieved through the efforts of two international working groups, namely, the Metadata and the Middleware Working Groups. An ILDG board with international representation supervises the work of these groups. The board chair rotates on an annual basis. To foster coordination, for the past five years the ILDG has held semiannual internet conferences through VRVS (Virtual Room Videoconferencing System) with worldwide participation.

Funding for this effort has been left to countries hosting the regional grids. For the most part funding has been minimal if not completely absent. The manpower, grid software, and necessary file storage capacity have been donated and/or borrowed from other funded projects. Nonetheless, over the course of five years, the ILDG has developed into a resource that is ready for use.

This is a brief status report. Rather than dwelling on the technical details of grid operation, I will try to take the perspective of a user.

2. Access policies

Lattice files in a grid repository may have access restrictions. These are set by the contributing collaboration. Thus it is always a good idea to check with the collaboration that created the files if you find there are restrictions. The authors are often comfortable releasing recent lattices selectively for noncompeting projects, or they might be willing to collaborate if there are overlapping interests. There is a spectrum of such policies ranging from permissive to more restrictive:

- All lattices are available as soon as they are generated (some collaborations).
- Recent lattices are available after negotiation (most collaborations).
- All lattices are available approximately six months after the first publication (universal).

Of course, in a publication based on another collaboration's lattices it is proper to cite an appropriate journal reference, where possible, and to acknowledge the collaboration that produced them.

It is very encouraging to note a historical trend toward increasing openness.

3. Files

The binary lattice files adhere to a prescribed format [4] called LIME [5]. (The name is a take-off on the name for the conventional MIME standard for e-mail, in this case meaning "lattice interchange message encapsulation"). The standard gives collaborations considerable leeway in adding their own variations. Essentially, the file consists of a series of records (messages), only three of which have required content: the main one, of course, is the binary payload. A second required message specifies the precision and space-time dimensions. A third contains the unique logical file name (LFN), for example,

```
lfn://USQCD/MILC/asqtad/2_plus_1_flavor/2064f21b676m007m050/  
series_1/l2064f21b676m007m050b.1530
```

The first part of the LFN (USQCD in this case) is a standardized prefix identifying the collaboration, and the rest is left to the discretion of the collaboration.

The logical file name (LFN) is used by the catalogs and file transfer utilities to identify the file. The mechanism works as follows: a user requests the file by naming its LFN. The retrieval software consults a replica catalog (RC), which associates the LFN with a universal resource locator (URL). The URL locates the file on the internet.

Each binary file is accompanied by a metadata file containing the archiving history, checksums and plaquette values, etc. Each ensemble of gauge configurations also has a metadata file containing information about the gauge action and the parameters used to generate it. Both types of metadata files are XML and must conform to a standard schema, collectively called QCDml. The Metadata Working Group sets all of these standards [6]. Please see Tomoteru Yoshie's poster contribution [7].

4. Mode of access

For a detailed account of file discovery and retrieval, please see Dirk Pleiter's poster contribution [8].

4.1 Grid certificates

Before you can download lattices you must obtain an X.509 grid certificate from an appropriate certificate authority (CA). The ILDG accepts certificates from any member of the ILDG Trust Federation [9]. Once you have a certificate, you must register it with the ILDG "virtual organization" [10].

4.2 Discovery

The obvious next step in accessing a set of lattices is to identify the ensemble(s) of interest. This is the purpose of the metadata catalog (MDC).

Each regional grid maintains a catalog of the files in its repository and publishes the MDC for those files. The regional grids then republish the contents of the world's catalogs through their web portals. This process is in various stages of development. Eventually all the regional grids will catalog the world's ensembles and be globally searchable.

A web-based global catalog is available in Australia (CSSM)[11], Europe (LDG)[12], Japan (JLDG)[13], and the US (JLab)[14]. Web-based search engines for searching the MDC's are also available in Australia and Japan. The UK provides a Java-based browser application to perform data discovery [15]. The United States currently has not populated its own MDC, but lattices in the older NERSC format continue to be available by means of a web interface through the Gauge Connection [1], and Brookhaven National Laboratory [16] has recently posted lattices from the RBC collaboration.

4.3 Downloading files

The final step involves the file transfer itself, which can proceed through various protocols directly (http or gridftp) or through the Storage Resource Manager (SRM v2) service framework. The latter allows client and server to negotiate the transfer protocol and endpoint that are actually used.

Client software is supposed to support SRM. The actual transfer protocol depends on the regional grid that dispenses the files. Australia, Japan and UK publish their data via a gridftp service. The JLDG additionally has a convenient web interface that provides the necessary download script [13]. The LDG dispenses files via SRM and provides a set of convenient tools called LTOOLS [17] to allow integrated access to their metadata, file catalogs, and storage elements. The UK uses its own set of free grid tools [15]. Finally, in the US, NERSC and BNL currently use http, but produce files only in the old NERSC format. An initial storage element is in development at FNAL, where there are now many files in ILDG format ready for SRM access and cataloging.

The middleware working group is working to alleviate this complex situation. Recently packages have been added to the LDG LTOOLS framework (which is relatively straightforward to install) that provide an SRM client (srmcp) and an initial version of an integrated client (ildg-client/ildg-get) that allows retrieval of metadata documents and files through http or SRM. This software, as well as the crucial catalogues such as the metadata and file catalogs are in the process of maturation, and the process should become better integrated and more reliable in the future.

5. What ensembles are or will soon be available?

I give a brief survey of some important and highly useful lattice ensembles now or soon to be available to the world community. As might be expected, they reflect a healthy diversity of approaches to lattice physics. I have not attempted an exhaustive list – rather I have included what I feel might be particularly interesting. Nor have I attempted to list all the important lattice parameters, such as lattice size and quark mass. The details are available in the meta data catalogs. There is such an impressive variety to choose from, surely there is something for every taste.

N_f	Action	Collaboration	a(fm)	cfs(approx)	Availability
0	tpLW	Adelaide	0.128	400	Available
2	FLIC'/tpLW	Adelaide	0.125	$400 \times \text{couple}$	In production

Table 1: Selected ensembles available through the Australian CSSM. The abbreviation “tpLW” stands for the tadpole Lüscher-Weiß action. For configuration number, the notation $400 \times n$ implies n ensembles of approximately 400 configurations each, typically with different choices of quark masses.

N_f	Action	Collaboration	a(fm)	cfs(approx)	Availability
2	NP-clover/Wilson plaq	QCDSF	0.07/0.11	5000×16	Negotiable
2	tmQCD/tlSym	ETMC	0.07/0.11	3500×15	Negotiable
$2 + 1$	stout/tpLW	QCDSF	0.08	1000×16	In progress
$2 + 1 + 1$	Stouted tmQCD/tlSym	ETMC	0.07/0.09	2500×15	In progress

Table 2: Selected ensembles available through the European LDG. Notation is the same as in previous tables. The abbreviation “tlSym” stands for the tree-level Symanzik gauge action. The abbreviation “tmQCD” stands for the twisted mass formulation.

5.1 Australia

The Adelaide group has only recently gained access to computing facilities that make it possible to begin serious unquenched calculations using the fat link irrelevant clover (FLIC) action. Production has begun as indicated in Table 1.

5.2 Europe

Europe (Table 2) has a couple of vigorous dynamical fermion efforts underway. The QCDSF collaboration has been generating some very large two-flavor ensembles based on the nonperturbative clover action and is following up with $2 + 1$ flavors of “stout” fermions. The ETMC has also been generating large two-flavor QCD ensembles with twisted mass fermions and plans to follow up with a full complement of flavors using a stouted version of the action.

5.3 Japan

In Japan (Table 3) the CP-PACS and JLQCD collaborations have access to very substantial computational resources, which have been devoted to two ambitious lattice generation projects using clover fermions and overlap fermions. The CP-PACS and JLQCD collaborations have recently released a significant set of full-QCD ensembles based on the Wilson-clover fermion action with the Iwasaki gauge action.

5.4 UKQCD and RBC Collaborations

Using QCDOC computers, the UKQCD collaboration has teamed up with the US RBC collaboration to generate a series of lattice ensembles based on the domain wall fermion formulation (Table 4). A large set has been released for general public access. A few of the most recent ensembles still have restricted access. The UKQCD has also been generating some full QCD lattices using the Asqtad formulation.

N_f	Action	Collaboration	$a(\text{fm})$	cfs(approx)	Availability
2	Clover/Iwasaki	CP-PACS	0.20	1000×4	Available
			0.15	1000×4	
			0.10	800×4	
2	Clover/Plaquette	JLQCD	0.10	1200×5	In preparation
$2 + 1$	Clover/Iwasaki	CP-PACS+ JLQCD	0.12	$800 \times 5 \times 2$	Available (new)
			0.10	$800 \times 5 \times 2$	
			0.07	$600 \times 5 \times 2$	
2	Overlap/Iwasaki	JLQCD	0.12	$O(500) \times 6$	After 1st spectrum paper

Table 3: Selected ensembles available through the Japanese JLDG. Notation is the same as in previous tables.

N_f	Action	Collaboration	$a(\text{fm})$	cfs(approx)	Availability
$2 + 1$	DWF/Iwasaki	UKQCD/RBC	0.12	800×4	Available
$2 + 1$	DWF/DBW2	UKQCD/RBC	0.12	300-1000	Available
2	DWF/DBW2	UKQCD/RBC	0.12	1000×3	Available
$2 + 1$	Asqtad/tpLW	UKQCD	0.12	3000	Available
$2 + 1$	DWF/Iwasaki	UKQCD/RBC	0.09	??	Restricted
$2 + 1$	DWF/Iwasaki	UKQCD/RBC	0.09	$?? \times 2$	In production

Table 4: Selected ensembles available through the UKQCD and RBC collaborations. Notation is the same as in previous tables. The question mark indicates the information was unknown at the time of this writing.

5.5 United States

In the US (Table 5) over the past few years the MILC collaboration has been generating and publishing an extensive set of full QCD ensembles based on the Asqtad formulation. The most recent additions are at a lattice spacing of 0.06 fm. Further work is underway to extend and add to the existing ensembles at 0.09 and 0.12 fm. All lattices are open to general access as soon as they are created. The LHPC collaboration has embarked on a major effort to generate dynamical clover ensembles on anisotropic lattices. The US RBC production of domain wall lattices was included in the previous section.

Acknowledgments

I am indebted to Balint Joo and Dirk Pleiter for checking over and contributing portions of the description of the middleware software operation.

References

- [1] The Gauge Connection: <http://qcd.nersc.gov/>.

N_f	Action	Collaboration	a(fm)	cfgs(approx)	Availability
2 + 1	Asqtad/tpLW	MILC	0.15	600 x 4	Available
2 + 1	Asqtad/tpLW	MILC	0.12	600 x 5	Available
2 + 1	Asqtad/tpLW	MILC	0.09	500 x 2	Available
				500 x 1	New, available
2 + 1	Asqtad/tpLW	MILC	0.06	500 x 2	In production Available
2 + 1	Aniso clover/tpLW	LHPC	0.125	500 x 4	Planned
2 + 1	Aniso clover/tpLW	LHPC	0.10	?? x 4	Planned
2 + 1	Aniso clover/tpLW	LHPC	0.08	?? x 4	Planned

Table 5: Selected ensembles available through the NERSC gauge connection or by contacting the collaborations directly. Notation is the same as in previous tables.

- [2] C. T. H. Davies, A. C. Irving, R. D. Kenway and C. M. Maynard [UKQCD collaboration], Nucl. Phys. Proc. Suppl. **119** (2003) 225 [arXiv:hep-lat/0209121]. ; A. C. Irving, R. D. Kenway, C. M. Maynard and T. Yoshie, Nucl. Phys. Proc. Suppl. **129** (2004) 159 [arXiv:hep-lat/0309029].
- [3] A. Ukawa, Nucl. Phys. Proc. Suppl. **140** (2005) 207 [arXiv:hep-lat/0409084]. ; K. Jansen, PoS(LAT2006)013 (2006) [arXiv:hep-lat/0609012].
- [4] ILDG file format:
<http://www-zeuthen.desy.de/~pleiter/ildg/ildg-file-format-1.1.pdf>.
- [5] LIME software and documentation: <http://usqcd.jlab.org/usqcd-docs/c-lime/>.
- [6] QCDml markup schema and examples: <http://www.ccs.tsukuba.ac.jp/ILDG/>;
<http://www.lqcd.org/ildg/>.
- [7] T. Yoshie, *Marking up lattice QCD configurations and ensembles*, these proceedings (2007).
- [8] D. Pleiter, *Towards an Interoperable International Lattice Datagrid*, these proceedings. (2007).
- [9] ILDG Trust Federation: <http://www.gridpma.org>.
- [10] Registration site for the ILDG virtual organization:
<https://grid-voms.desy.de:8443/vo/ildg/vomrs/>.
- [11] CSSM portal: <http://cssm.sasr.edu.au/ildg/>.
- [12] LDG portal: <http://www-zeuthen.desy.de/latfor/>.
- [13] JLDG portal: <http://www.jldg.org/lqa/index.html>.
- [14] JLab MDC portal: <http://usqcd.jlab.org/mdc-web-client/index.jsp>.
- [15] DiGS software: <http://forge.nesc.ac.uk/projects/qcdgrid/>.
- [16] Domain wall fermion lattices from the RBC collaboration: <https://qcdlattices.bnl.gov/>.
- [17] LTOOLS software for the LDG: <http://www-zeuthen.desy.de/latfor/ldg/doc/>.

Heavy baryon mass spectrum from lattice QCD with 2+1 dynamical sea quark flavors

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We investigate the mass differences of charm and bottom heavy baryons, using MILC lattice gauge configurations with 2+1 dynamical sea quark flavors. We extend our previous work to three lattice spacings: fine ($a \approx 0.09$), coarse ($a \approx 0.12$), and medium-coarse ($a \approx 0.15$) ensembles. For extrapolations and interpolations, we apply simultaneous quadratic fits and simple linear fits with the full QCD data points for the valence quark masses as well as the sea quark masses.

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1. Introduction

Heavy baryons have been investigated by both experimental and theoretical approaches. From experiment, the singly charmed heavy baryon mass spectrum is well known; however, the other heavy baryon masses are only crudely known. Recently, mass measurements of the singly bottom baryon Ξ_b^- have been published by the D0 [1] and CDF [2] collaborations. From lattice QCD, there are several quenched calculations [3–8] and dynamical sea quark flavor simulations [9–11] for the heavy baryon mass spectrum, and most results are in fair agreement with observed values. In this work, we extend our previous dynamical sea quark flavor simulation [9][10] with a larger data set and more systematic analysis methods.

We use the MILC fine ($a \approx 0.09$), coarse ($a \approx 0.12$), and medium-coarse ($a \approx 0.15$) lattices [12]. We apply two local interpolating operators [3] and construct heavy baryon two point functions with improved clover heavy quark propagators with the Fermilab interpretation [13] and improved staggered light quark propagators. We extract the mass differences from the ratio of propagators and extrapolate to the chiral limit using simultaneous quadratic fits and simple linear fits with the full QCD data points.

2. Formalism

We used two types of interpolating operators [3] for the singly heavy baryons, which are

$$\mathcal{O}_5 = \varepsilon_{abc}(\psi_1^{aT} C \gamma_5 \psi_2^b) \Psi_H^c \quad \text{and} \quad \mathcal{O}_\mu = \varepsilon_{abc}(\psi_1^{aT} C \gamma_\mu \psi_2^b) \Psi_H^c, \quad (2.1)$$

where ε_{abc} is the Levi-Civita tensor, ψ_1 and ψ_2 are light valence quark fields for up, down, or strange quarks, Ψ_H is the heavy valence quark field for the charm or the bottom quark, C is the charge conjugation matrix, and a , b , and c are color indices. Basically, $\mathcal{O}_5$ is the operator for $s^\pi = 0^+$ and $\mathcal{O}_\mu$ is for $s^\pi = 1^+$, where s^π is the spin parity state of the light quark pair. Therefore, $\mathcal{O}_5$ describes total spin $J = \frac{1}{2}$ baryons (Λ_H , Ξ_H), and $\mathcal{O}_\mu$ describes $J = \frac{1}{2}$ baryons (Σ_H , Ξ'_H , Ω_H) as well as $J = \frac{3}{2}$ baryons (Σ_H^* , Ξ_H^* , Ω_H^*). For doubly heavy baryons, we can simply interchange the heavy quark field and the light quark fields in Eq. 2.1 [5].

We apply the method of Wingate *et al.* [14] to combine staggered propagators for the light valence quarks and a Wilson type (clover) propagator for the heavy valence quark. Since we use staggered light quarks, we needed to consider taste mixing. In our previous work [10][15], we found that there is no taste mixing between the light quarks. However, due to cancellations among the copy indices, we cannot separate spin $J = \frac{1}{2}$ and $J = \frac{3}{2}$ states from the operator $\mathcal{O}_\mu$ using standard spin projection operators.

3. Data analysis

Since we use the Fermilab interpretation [13] for the heavy quarks, the absolute mass from the simulation is not a physical quantity. The physical mass M_{phy} of the baryon is

$$M_{phy} = M_{cal} + \Delta, \quad (3.1)$$

where M_{cal} is the simulation result and Δ is a constant mass shift. We can calculate the constant mass shift from calculations of the kinetic mass with non-zero momenta or heavy-light meson spectroscopy. In this project, however, we estimate mass differences, which are directly measurable quantities without determining Δ .

Since we are interested in mass differences, we can take the ratio of two propagators and fit the mass difference directly. A fit model function $P_r(t)$ of the ratio of the propagators is

$$P_r(t) = \frac{A_1 e^{-m_1 t} + \dots}{A_2 e^{-m_2 t} + \dots} = A'_1 e^{-(m_1 - m_2)t} + \dots \quad (3.2)$$

Since the propagators are calculated using the same gauge configurations, the propagators in numerator and denominator are correlated with each other. Using this method, we expect smaller statistical errors and more stable fits.

We can take the ratio of the propagators, for example, between Ξ'_c and Λ_c ,

$$C_r(t) = \frac{\sum_{k=1}^N C_k^{\Xi'_c}(t)}{\sum_{k=1}^N C_k^{\Lambda_c}(t)} = \frac{\bar{C}^{\Xi'_c}(t)}{\bar{C}^{\Lambda_c}(t)}, \quad (3.3)$$

where k is the configuration index. The covariance matrix of the ratio is estimated using bootstrap sampling.

We display an example of this method for Ξ'_c and Λ_c on the fine lattice with dynamical quark masses $m_l = 0.4m_s$ and 0.0062 light valence quark mass in Fig. 1. The jittery pattern appears strongly in the ratio (Fig. 1 (a)), because the opposite parity state contributions are substantially different for numerator and denominator. In fact, Ξ'_c contains large opposite parity state contributions, while Λ_c contains very weak opposite parity state contributions.

We obtained the most reasonable fit from a fit model function with one non-alternating phase exponential and one alternating phase exponential. That fit is shown in Fig. 1(b). The maximum distance of the fit is $D_{\max} = 22$ and a plateau appears where $D_{\min} \geq 8$.

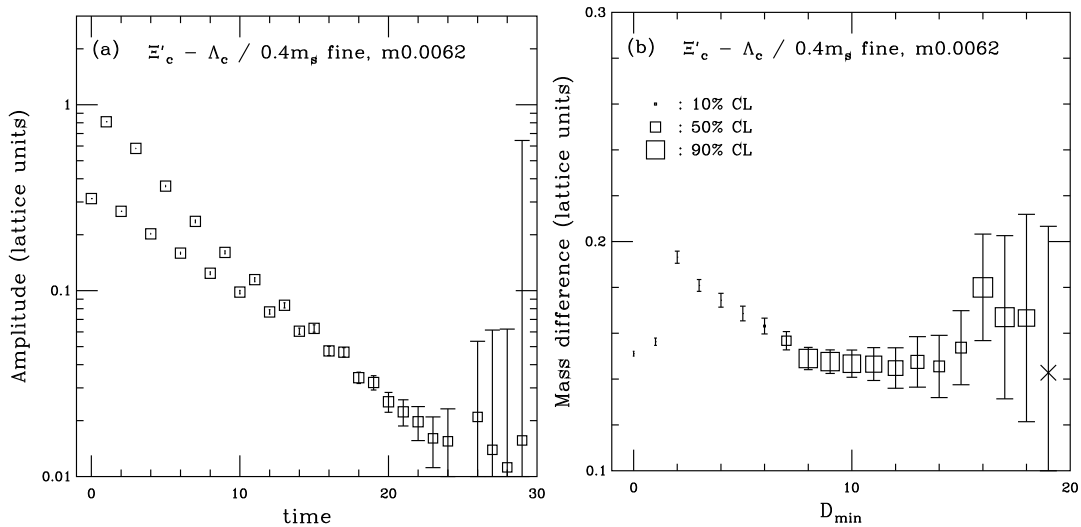


Figure 1: The ratio of the propagators (a) and the two particle fit of the ratio (b). The size of the symbols on (b) is proportional to the confidence level (CL).

The mass difference can also be obtained by first fitting the propagators individually, and then subtracting the masses to obtain the difference. We can compare this method shown in Fig. 2 to the ratio method. As we expected, the individual mass fits for Ξ'_c and Λ_c (Fig. 2) are worse than the fit of the ratio (Fig. 1 (b)). For Ξ'_c , the confidence levels are fine; however, the fluctuation of the plateau is larger (the systematic error is larger), and for Λ_c , fits are not stable. From this comparison, we conclude that the ratio method is better.

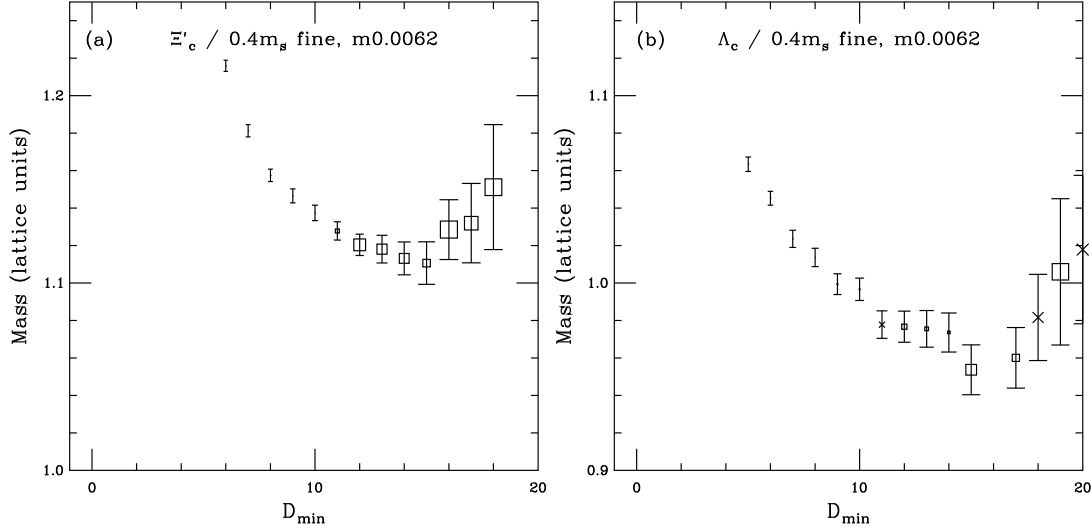


Figure 2: The individual fits for Ξ'_c (a) and Λ_c from the propagators. The square symbols indicate successful fits and the cross symbols indicate unstable fits. The size of the symbols is proportional to the confidence level. We obtained these fits from a fit model function with one non-alternating phase exponential and one alternating phase exponential.

Once we obtain the mass differences, we need to perform extrapolations to the physical quark mass. In this analysis, we extrapolate the valence quark masses and the sea quark masses simultaneously, using a quadratic fit model function given by

$$P_{\text{quad}} = c_0 + c_1 m_l + c_2 m_l^2 + c_3 m_s + c_4 m_{\text{sea}} \quad (3.4)$$

where c_0 to c_4 are the fitting parameters, m_l is the light valence quark mass, m_s is the strange valence quark mass, and m_{sea} is the light sea quark mass. We fixed $c_3 = 0$ except for the coarse lattice, since only the coarse lattice has multiple (three) strange valence quark masses. We would prefer to use a heavy baryon mass formula based on partially quenched chiral perturbation theory, but do not know of one. We can also perform the extrapolations with only the full QCD data points, *i.e.*, the points for which the valence quark masses match the corresponding sea quark masses. In general, the errors of the full QCD extrapolations are larger than those of the simultaneous quadratic fits, because the simultaneous fit uses more data to constrain the fit parameters.

4. Results and discussion

Parameters of the ensembles [12] are summarized in Table 1. The scale of each ensemble was

a (fm)	am_l/am_s	L (fm)	β	size	r_1/a	# confs
~ 0.15	0.0097 / 0.0484	2.4	6.572	$16^3 \times 48$	2.1356	631
~ 0.15	0.0194 / 0.0484	2.4	6.586	$16^3 \times 48$	2.1284	631
~ 0.15	0.0290 / 0.0484	2.4	6.600	$16^3 \times 48$	2.1245	440
~ 0.12	0.007 / 0.05	2.4	6.76	$20^3 \times 64$	2.6349	545
~ 0.12	0.01 / 0.05	2.4	6.76	$20^3 \times 64$	2.6183	590
~ 0.12	0.02 / 0.05	2.4	6.79	$20^3 \times 64$	2.6477	452
~ 0.09	0.0062 / 0.031	2.4	7.09	$28^3 \times 96$	3.7016	534
~ 0.09	0.0124 / 0.031	2.4	7.11	$28^3 \times 96$	3.7138	557

Table 1: MILC lattice parameters. The three nominal lattice spacings in the first column (0.15, 0.12, and 0.09 fm) correspond to medium-coarse, coarse, and fine ensembles, respectively. The bare light (strange) sea quark mass in lattice units is am_l (am_s). The spatial size of the lattice is L and $\beta = 10/g^2$, where g is the bare gauge coupling. In the sixth column we show r_1/a calculated from a global fit to r_1 values on all our ensembles [16].

determined by a length scale r_1 from the static quark potential using f_π as an input parameter [17]:

$$r_1 = 0.3108(15)(^{+26}_{-79})\text{fm}. \quad (4.1)$$

We present mass splittings in MeV for singly heavy baryons in Fig. 3. We investigate five $J^P = \frac{1}{2}^+$ singly heavy baryons (Λ_H , Ξ_H , Σ_H , Ξ'_H , Ω_H). There are ten possible mass splitting combinations. Since not all of the combinations are independent and all dependent combinations are consistent each other, we display only four independent combinations on the figure. We display the comparison of the singly charmed baryons and the PDG data [18] in Fig. 3 (a). The error bars of our calculations are larger than those of experiment, but smaller than or comparable to those of previous lattice calculations [3–8]. For the singly bottom baryons in Fig. 3 (b), we compare with experimental results measured by the CDF and D0 collaborations [1][2] and a dynamical calculation result by Lewis and Woloshyn [11]. Our error bars, in general, are smaller than those of Lewis and Woloshyn, especially for the fine lattice result.

Since the singly charmed baryons are experimentally well known, let us examine more closely our singly charm results. The mass differences between $\Xi_c - \Lambda_c$, $\Xi'_c - \Sigma_c$, and $\Omega_c - \Xi'_c$ are in good agreement with the PDG data [18]; however, the mass difference $\Omega_c - \Lambda_c$ is not. Note that Λ_c and Ξ_c are calculated from the operator $\mathcal{O}_5$, and Σ_c , Ξ'_c , and Ω_c are calculated from the operator $\mathcal{O}_\mu$. Thus, the disagreement occurs on the mass differences of the heavy baryons that come from the different operators. On the fine lattice result, especially, this pattern is quite evident. We checked the other mass differences with the different operator combinations, and we obtained similar discrepancies from the PDG data [18]. We hope that this can be resolved by studying the constant mass shift due to the heavy quarks or the hyper-fine structure of the singly heavy baryons. Resolving this puzzle is a high priority.

We also present the doubly charmed and bottom baryons in Fig. 4. We display our fine and coarse lattice results with those of Lewis *et al.* [4] for the doubly charmed baryons and Lewis and Woloshyn [11] with dynamical sea quarks for the doubly bottom baryons. We set the scale of the

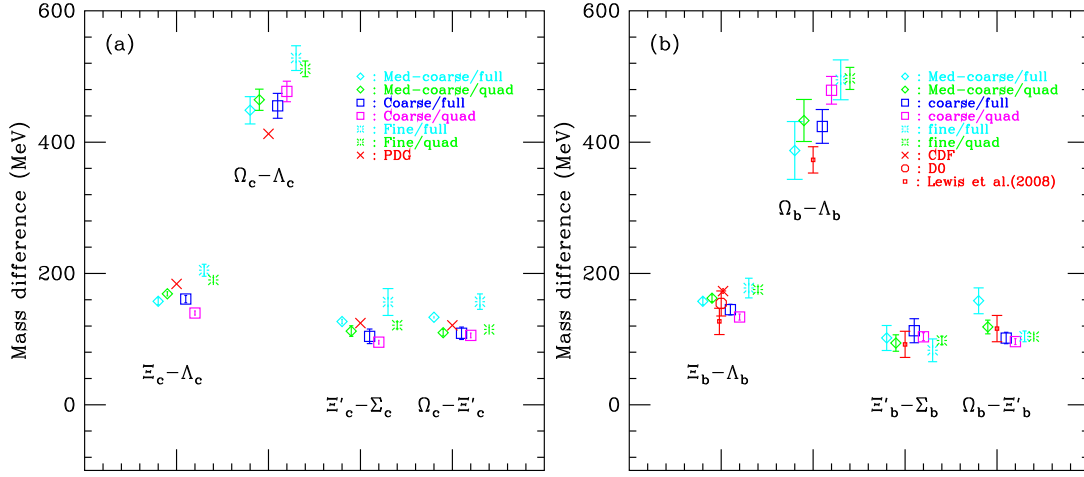


Figure 3: Independent mass differences of $J^P = \frac{1}{2}^+$ singly charmed baryons (a), and singly bottom baryons (b). In the legend, “full” indicates the full QCD data point fit result, and “quad” indicates the simultaneous quadratic fit result.

y-axis of the figure from the other group’s results, because they calculated the absolute masses, while we calculated the static masses. For the doubly charmed baryons, we added 193 and 438 MeV, and for the doubly bottom baryons, we added 2.833 and 4.223 GeV to our fine and coarse lattice results, respectively. Our results agree fairly well with prior results. The mass differences between Ξ_{HH} and Ω_{HH} are about 100 MeV, which is about the strange quark mass. The hyper-fine splittings are about 30 ~ 80 MeV. Moreover, the hyper-fine splittings of the doubly bottom baryons are smaller than those of the doubly charmed baryons, because of heavy quark symmetry.

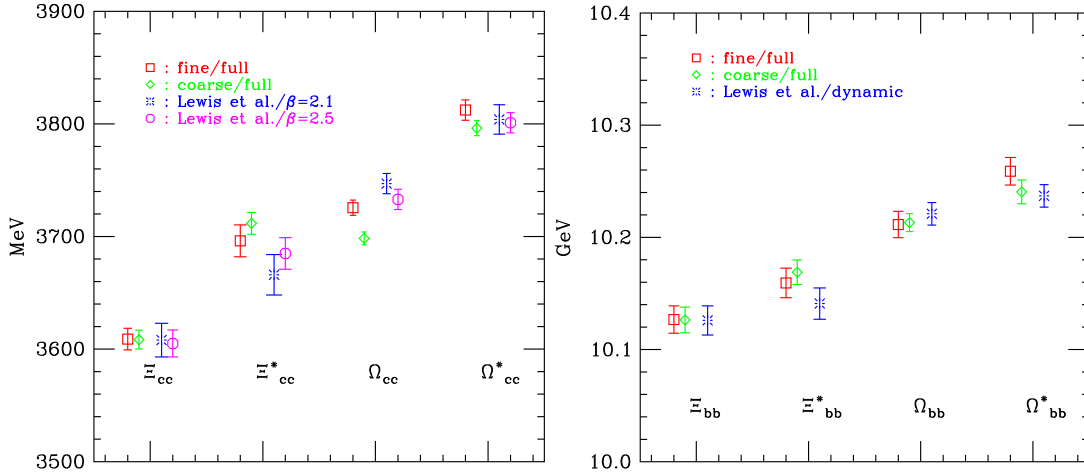


Figure 4: The mass spectrum of doubly charmed and bottom baryons. The error bars are statistical only.

Acknowledgments

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References

- [1] A.M.Abazov *et al.*, *Phys. Rev. Lett.* **99** (2007) 052001.
- [2] T. Aaltonen *et al.*, *Phys. Rev. Lett.* **99** (2007) 052002.
- [3] K.C. Bowler *et al.* (UKQCD Collaboration), *Phys. Rev. D* **54** (1996) 3619.
- [4] R. Lewis *et al.*, *Phys. Rev. D* **64** (2001) 094509.
- [5] N. Mathur *et al.*, *Phys. Rev. D* **66** (2002) 014502.
- [6] S. Gottlieb and S. Tamhankar, *Nucl. Phys. Proc. Suppl.* **119** (2003) 644.
- [7] A. Ali Khan *et al.*, *Phys. Rev. D* **62** (2000) 054505.
- [8] J. M. Flynn *et al.*, *JHEP* **7** (2003) 66.
- [9] H. Na and S. Gottlieb, PoS(LAT2006)191 [hep-lat/0610009].
- [10] H. Na and S. Gottlieb, PoS(LAT2007)124, arXiv:0710.1422 [hep-lat]
- [11] R. Lewis and R. M. Woloshyn, arXiv:0806.4783 [hep-lat]
- [12] C. Aubin *et al.*, *Phys. Rev. D* **70** (2004) 094505.
- [13] A. El-Khadra, A. Kronfeld, and P. Mackenzie, *Phys. Rev. D* **55** (1997) 3933.
- [14] M. Wingate *et al.*, *Phys. Rev. D* **67** (2003) 054505.
- [15] S. Gottlieb, H. Na, and K. Nagata, *Phys. Rev. D* **77** (2008) 017505, arXiv:0707.3537 [hep-lat].
- [16] D. Toussaint, *Private communication*.
- [17] C. Bernard *et al.*, PoS(LAT2007)090.
- [18] W.M. Yao *et al.*, *J. Phys. G* **33** (2006) 1.

HISQ action in dynamical simulations

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We report on recent progress in employing the Highly Improved Staggered Quark (HISQ) action introduced by the HPQCD/UKQCD collaboration in simulations with dynamical fermions. The HISQ action is an order a^2 Symanzik-improved action with further suppressed taste symmetry violations. The improvement in taste symmetry is achieved by introducing Fat7 smearing of the original gauge links and reunitarization (projection to an element of $U(3)$ or $SU(3)$) followed by Asq-type smearing. Major challenges for calculating the fermion force are related to the reunitarization step. We present a preliminary study of the HISQ action on two 2+1+1 flavor ensembles with the lattice spacing roughly equivalent to the MILC asqtad $a = 0.125$ and 0.09 fm ensembles.

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1. Introduction

The Highly Improved Staggered Quark (HISQ) action developed in Ref. [1] is an $O(a^2)$ Symanzik-improved action for which additional suppression of taste-exchange interactions is achieved by replacing the original gauge links U in the Dirac operator by

$$U \rightarrow X = \mathcal{F}_2 \mathcal{U} \mathcal{F}_1 U \quad (1.1)$$

where intermediate sets of links V, W, X are defined as

- $\mathcal{F}_1$ – smearing level 1 (Fat 7): $V = \mathcal{F}_1 U$,
- $\mathcal{U}$ – reunitarization: $W = \mathcal{U} V$,
- $\mathcal{F}_2$ – smearing level 2 (Asq): $X = \mathcal{F}_2 W$.

A new feature of the HISQ action compared with asqtad is the reunitarization step that gives an extra contribution to the fermion force.

2. Fermion force and reunitarization

In molecular dynamics simulations we are sampling an ensemble of gauge configurations weighted by $\exp(-S)$, where the action $S = S_g + S_f$ is split into gauge, S_g , and fermionic, S_f , parts. As usual, the integration over Grassmann variables is performed and then a set of pseudo-fermion fields Φ is introduced, resulting in the fermionic part of the form $S_f \sim \langle \Phi | (M^\dagger(U) M(U))^{-N_f/4} | \Phi \rangle$. One can consult the details of the algorithm in [2] and recent ideas on efficient evaluation of the fermion force for HISQ in [3].

The fermion force is calculated by taking the derivative of the action S_f with respect to fundamental gauge links U using the chain rule along the lines of Refs. [3], [4]. Schematically:

$$\frac{\partial S_f}{\partial U} = \frac{\partial S_f}{\partial X} \frac{\partial X}{\partial W} \frac{\partial W}{\partial V} \frac{\partial V}{\partial U} . \quad (2.1)$$

The following parts are the same as for the asqtad action: $\partial S_f / \partial X$, $\partial X / \partial W$, $\partial V / \partial U$, while the contribution from the reunitarization step $\partial W / \partial V$ is new.

We have experimented with projecting to SU(3) and U(3) groups and found that pion spectrum measurements with valence HISQ and sea asqtad quarks show no difference, as one would expect on physical grounds. Therefore in our dynamical HISQ simulations we always perform projection to the group U(3). While keeping the physics the same, this has two advantages:

1. Different methods of projection, namely polar decomposition and trace maximization, give identical results. (The same is not true in the SU(3) case.)
2. When projecting from U(3) to SU(3) by making the determinant of the matrix equal to 1, one needs to choose among three possibilities for the phase. In dynamical simulations one needs to track this phase to make sure it changes smoothly for each link. Otherwise discontinuous changes lead to rapid changes in the action similar to those we describe below.

We adopt the following method of U(3) projection. For a complex matrix V the matrix $H = V^\dagger V$ is Hermitian and $W = VH^{-1/2}$ is unitary. We first calculate $H^{-1/2}$ by using the Cayley-Hamilton theorem in a manner similar to the approach in Refs. [5], [6]:

$$H^{-1/2} = f_0 \mathbb{I} + f_1 H + f_2 H^2, \quad (2.2)$$

where f_i are functions of $c_i = \text{Tr}(H^{i+1})/(i+1)$, $i = 0, 1, 2$. To evaluate the derivative of $H^{-1/2}$ with respect to H one needs to know the derivative of f_i with respect to H . This can be performed analytically by applying the chain rule and making use of the coefficients explicitly calculated in Ref. [6]. After $\partial H^{-1/2}/\partial H$ is known we have trivially:

$$\frac{\partial W}{\partial V} = \frac{\partial V}{\partial V} H^{-1/2} + V \frac{\partial H^{-1/2}}{\partial H} \frac{\partial H}{\partial V}. \quad (2.3)$$

(We write Eq. (2.3) schematically, but in fact each matrix-matrix derivative is a rank 4 tensor with indices contracted in such a way that the resulting expression on the right hand side is a rank 4 tensor again. An excellent review on how to deal with such derivatives can be found in [4].) Thus the entire derivation can be performed analytically. (We also implemented a finite difference scheme and rational function approximation but found them much less accurate than the procedure described here.)

To understand the possible behaviour of $\partial W/\partial V$ qualitatively let us consider the U(1) case for the moment. Then $V = r e^{i\theta}$ and $W = V(V^\dagger V)^{-1/2} = e^{i\theta}$, and the derivative

$$\frac{\partial W}{\partial V} = \left(\frac{\partial W}{\partial V} \right)_{V^\dagger} = \frac{\partial(W, V^\dagger)}{\partial(V, V^\dagger)} = \frac{\partial(W, V^\dagger)}{\partial(r, \theta)} \frac{\partial(r, \theta)}{\partial(V, V^\dagger)} = \frac{1}{2r} \quad (2.4)$$

is large when r is small, as might happen when the links U are locally disordered, and the first stage of smearing results in a small smeared link V . For the matrix case the derivative is dominated by the smallest eigenvalue of V . To derive Eq. (2.4) we applied the method of Jacobians and the notation is similar to the one used in Thermodynamics.

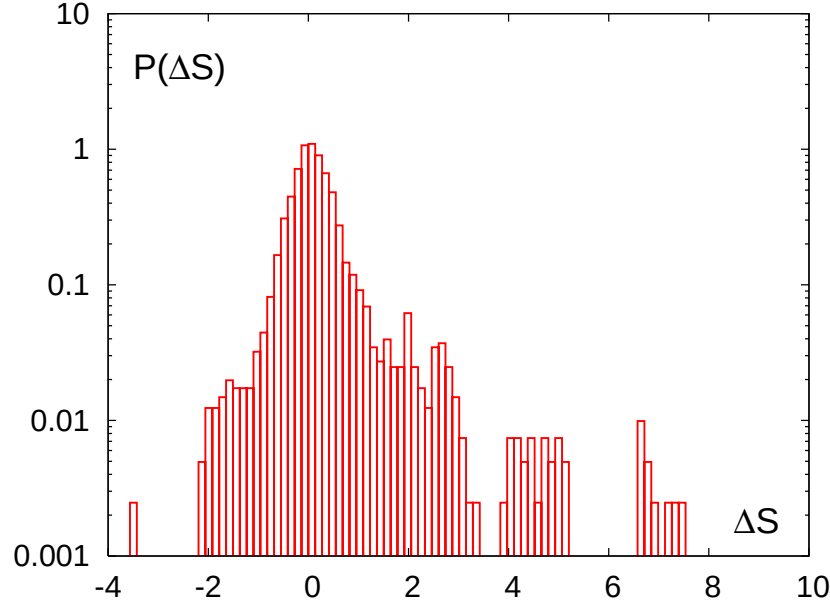
3. Dynamical HISQ simulations

We run the RHMC algorithm with five pseudofermion fields. The first pseudofermion implements the ratio of the determinants for two light and one strange quark to the determinant for three unphysical heavy quarks (“UHQ”) with mass $am_{\text{UHQ}} = 0.2$. The next three each implement the determinant for one UHQ, and the final pseudofermion implements a physical charm quark, including the mass correction to the Naik term to first order in m .

At the time we did our studies, one loop fermion corrections to the gauge action were not yet known, so we used the coefficients in our gauge action appropriate for the asqtad fermion action. (The coefficients of the gauge action with 1-loop corrections due to HISQ have been calculated and are now available [8].)

Our integration algorithm is the “3G1F” (“three gauge steps, one fermion step”) algorithm, with the Omelyan integrator used for both gauge and fermion forces. Our convention for the step size is that each application of the fermion force is one step. Note that since the Omelyan integrator shifts the time at which the force is calculated alternately forward and backward, the full period in

$N_s^3 \times N_t$	Conf.	β	am_l	am_s	am_c	Δt	a , fm
$20^3 \times 64$	40	6.75	0.010	0.050	0.600	0.04167	0.127
$28^3 \times 96$	50	7.07	0.007	0.035	0.420	0.03125	0.093
$48^3 \times 144$	6	7.47	0.004	0.020	0.240	0.01250	0.060

Table 1: Dynamical HISQ 2+1+1 ensembles.**Figure 1:** The histogram of the change in the action.

simulation time of the integrator is twice what we call the step size. For example, when we run a fifty-step trajectory this means 25 cycles of the Omelyan integrator, involving 50 fermion force calculations and 150 gauge force calculations. The parameters of the three 2+1+1 flavor ensembles we have run are compiled in Table 1. The lattice spacing is calculated by measuring the ratio r_1/a from the static quark potential and using the value $r_1 = 0.318$ fm [7].

While most trajectories ran smoothly, we found many trajectories with large jumps in the action as the integration proceeded. In Fig. 1 we show the histogram of the change in the action, plotted on a logarithmic scale, over several time units for the $a = 0.127$ fm ensemble. The long tail “outliers” indicate instantaneous jumps in the action, which we investigate further.

Let us denote the norm of a matrix A by:

$$||A|| = \sqrt{\sum_{i,j} |A_{ij}|^2}.$$

When we calculate the fermion force at each time step as an anti-Hermitian matrix defined on each link, we evaluate its norm and find the maximum value over the lattice: $||F||_{max}$. Also, at each time step we calculate the determinant of V (Fat7 smeared) links and find the minimum value over the lattice: $|\det V|_{min}$. Time histories of these two quantities are shown in Fig. 2. Large values of the

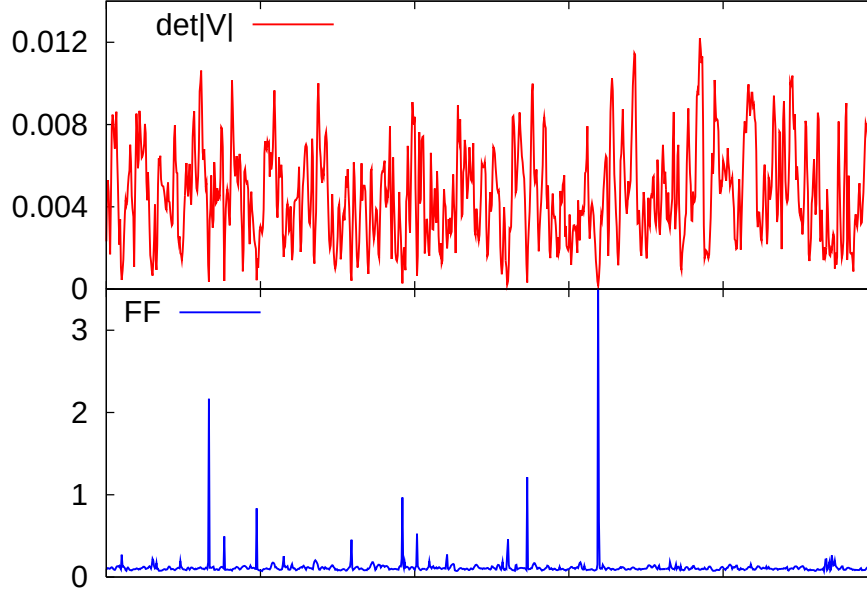


Figure 2: The time history of $|\det V|_{min}$ (top) and $||F||_{max}$ (bottom) for the $a = 0.127$ fm ensemble during 5 time units ($= 5 \times 24 = 120$ time steps).

fermion force accompany small values of the determinant (or small eigenvalues) of Fat7 smeared links. Thus, when calculating smeared links by adding different paths one may by chance produce a matrix V with an eigenvalue close to 0, which in turn leads to a large derivative dW/dV (as in the U(1) example considered earlier) that results in a large fermion force. Our integration algorithm has a finite step size, so it is not able to integrate such “spikes” in the force smoothly, leading to instantaneous jumps in the action that we see as “outliers” in the action histogram Fig. 1.

We investigated how this situation changes when we go to finer (smaller lattice spacing) ensembles. Since configurations become smoother, spikes in the force become less severe, as seen in Fig. 3.

4. Pion splittings on dynamical HISQ configurations

The effect of suppression of the taste-exchange interactions in HISQ was investigated in [1] by measuring the pion spectrum with valence HISQ on sea asqtad configurations. Here we report on similar measurements performed on dynamical HISQ configurations for the first two ensembles of Table 1.

It is convenient to define a dimensionless quantity which is almost independent of quark mass:

$$\Delta \equiv (M_\pi^2 - M_G^2)r_1^2, \quad (4.1)$$

where M_G corresponds to the Goldstone pion and M_π refers to one of the other seven pion tastes in Tables 2 and 3. We calculate Δ for comparable asqtad and HISQ configurations, and then the ratio

$$R \equiv \frac{\Delta_{ASQ}}{\Delta_{HISQ}} \quad (4.2)$$

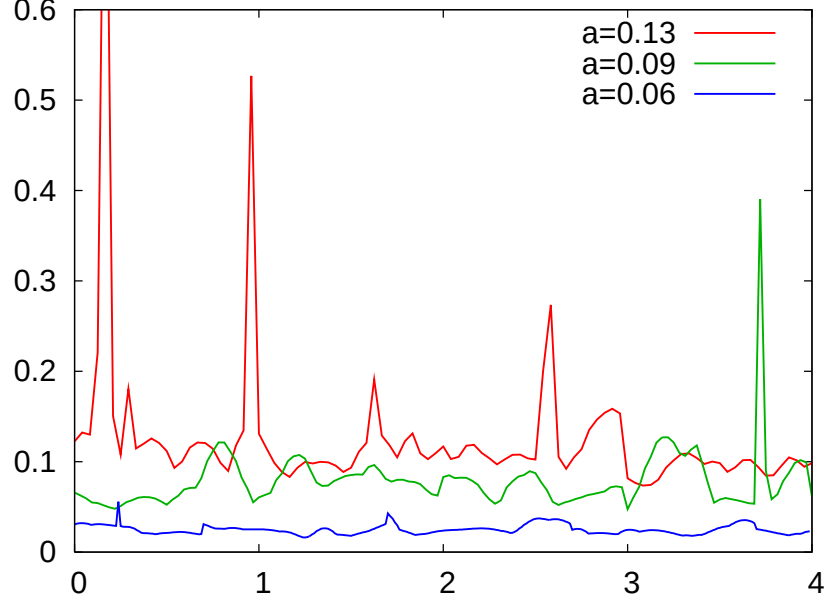


Figure 3: Fermion force $||F||_{max}$ for different ensembles versus time in time units (1 time unit corresponds to 24 steps for $a = 0.127$, 32 steps for $a = 0.093$ and 80 steps for $a = 0.060$ ensemble).

Pion taste	$r_1 M_\pi^{ASQ}(658)$	$r_1 M_\pi^{HISQ}(40)$	Δ_{ASQ}	Δ_{HISQ}	R
γ_5	0.2244(02)	0.1889(07)			
$\gamma_0 \gamma_5$	0.2815(11)	0.2071(27)	0.029(1)	0.0072(11)	4.0(6)
$\gamma_i \gamma_5$	0.2822(05)	0.2058(10)	0.029(0)	0.0067(05)	4.4(3)
$\gamma_i \gamma_j$	0.3134(20)	0.2224(33)	0.048(1)	0.0138(15)	3.5(4)
$\gamma_i \gamma_0$	0.3126(11)	0.2188(19)	0.047(1)	0.0122(08)	3.9(3)
γ_i	0.3347(28)	0.2306(56)	0.062(2)	0.0175(26)	3.5(5)
γ_0	0.3373(15)	0.2311(22)	0.063(1)	0.0178(10)	3.6(2)
$\mathbb{I}$	0.359(5)	0.252(12)	0.079(4)	0.0280(61)	2.8(6)

Table 2: Pion spectrum on $a = 0.127$ fm HISQ ensemble.

shows how much the splittings decrease when going from asqtad to HISQ. The values of R for different pion tastes are shown in the last column of Tables 2 and 3. The statistical errors are rather large since for HISQ we have about an order of magnitude fewer configurations than for asqtad. The number of configurations used for measurements is indicated in parentheses in the headers of the second and third column. The overall trend is however clear and in agreement with Ref. [1]: about a factor of three improvement in taste symmetry for the HISQ action relative to asqtad.

5. Conclusions

In dynamical HISQ simulations with typical parameters, we found that smearing may produce a smeared link V with a small eigenvalue that dominates the derivative of the reunitarized link W ,

Pion taste	$r_1 M_\pi^{\text{ASQ}}(572)$	$r_1 M_\pi^{\text{HISQ}}(50)$	Δ_{ASQ}	Δ_{HISQ}	R
γ_5	0.2069(05)	0.1378(08)			
$\gamma_0 \gamma_5$	0.2177(10)	0.1420(08)	0.0046(5)	0.0012(4)	4(1)
$\gamma_i \gamma_5$	0.2187(07)	0.1428(08)	0.0050(4)	0.0014(3)	3.6(8)
$\gamma_i \gamma_j$	0.2256(11)	0.1467(21)	0.0081(5)	0.0025(7)	3.2(8)
$\gamma_0 \gamma_0$	0.2259(07)	0.1475(11)	0.0082(4)	0.0028(4)	3.0(4)
γ_i	0.2311(15)	0.1485(16)	0.0106(7)	0.0031(5)	3.5(6)
γ_0	0.2318(10)	0.1509(11)	0.0109(5)	0.0038(4)	2.9(3)
$\mathbb{I}$	0.2398(25)	0.1522(27)	0.015(1)	0.0042(9)	3.5(8)

Table 3: Pion spectrum on $a = 0.093$ fm HISQ ensemble.

dW/dV , and gives a large contribution to the fermion force. Such “spikes” in the force integrated with finite time steps give “jumps” in the action that decrease the acceptance rate of the RHMC algorithm. This problem was noted in Ref. [6] and is probably related to topological defects, “dislocations” that manifest themselves in plaquettes with low values lying on the tails of the plaquette distribution. We found that going to finer ensembles (smoother gauge configurations) reduces the number of spikes and partially cures the problem.

On configurations generated with the HISQ action for dynamical quarks we measured the staggered pion spectrum and found that pion splittings decrease by a factor of three or more, confirming the result of Ref. [1], where pioneering tests were done with valence HISQ fermions on configurations with asqtad sea quarks.

References

- [1] E. Follana, Q. Mason, C. Davies, K. Hornbostel, G.P. Lepage, J. Shigemitsu, H. Trottier and K. Wong, Phys. Rev. D **75**, 054502 (2007) [arXiv:hep-lat/0610092v1].
- [2] S. Gottlieb, W. Liu, D. Toussaint, R. L. Renken and R. L. Sugar, Phys. Rev. D **35**, 2531 (1987).
- [3] K. Y. Wong and R. M. Woloshyn, PoS(LAT2007) 047, 2007 [arXiv:0710.0737 [hep-lat]].
- [4] W. Kamleh, D. B. Leinweber and A. G. Williams, Phys. Rev. D **70**, 014502 (2004) [arXiv:hep-lat/0403019].
- [5] C. Morningstar and M. J. Peardon, Phys. Rev. D **69**, 054501 (2004) [arXiv:hep-lat/0311018].
- [6] A. Hasenfratz, R. Hoffmann and S. Schaefer, JHEP **0705**, 029 (2007) [arXiv:hep-lat/0702028].
- [7] C. Aubin, C. Bernard, C. DeTar, Steven Gottlieb, E.B. Gregory, U.M. Heller, J.E. Hetrick, J. Osborn, R. Sugar, D. Toussaint, Phys. Rev. D **70**, 094505 (2004) [arXiv:hep-lat/0402030].
- [8] A. Hart, G.M. von Hippel and R.R. Horgan, these proceedings.

Progress on four flavor QCD with the HISQ action

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We describe recent progress on generation of gauge configurations using the Highly Improved Staggered Quark (HISQ) action that was designed by the HPQCD/UKQCD collaboration. The HISQ action requires two levels of smearing with a reunitarization of the links before the second smearing. We describe how we deal with the occurrence of occasional large forces arising from the reunitarization step. The MILC collaboration is currently generating ensembles with approximate lattice spacings of 0.15, 0.12, 0.09, and 0.06 fm, with the strange and charm quark masses close to their physical values and the mass of the light quarks m_l set to $0.2m_s$. We present recent results for pion taste splittings, light hadron masses, the static potential, the η_c dispersion relation and the topological susceptibility.

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1. Introduction

The MILC collaboration has been using the asqtad action [1] for more than a decade for its generation of 2+1 flavor dynamical quark configurations. Over forty ensembles covering six lattice spacings from $a \approx 0.18$ fm to 0.045 fm and a wide range of quark masses have enabled us to explore both the continuum and chiral limits [2].

Recently, the Highly Improved Staggered Quark (HISQ) [3] action was developed by the HPQCD/UKQCD collaboration. This action requires two levels of smearing with a reunitarization of the links before the second smearing. Although it is more expensive to simulate than the asqtad action, its reduced taste symmetry breaking makes the HISQ action an attractive possibility for future calculations. It also allows us to include a dynamical charm quark with reasonable accuracy at current lattice spacings. The goal of this initial work is to generate several ensembles with a fixed ratio of light to strange quark masses and to study the approach to the continuum limit.

Large forces arise during molecular dynamics updating when the determinant of a link at the first level of smearing is close to vanishing [4]. This problem is dealt with by a slight change in the guiding action, the effect of which can be eliminated via the accept/reject step at the end of each trajectory.

The MILC collaboration is currently generating ensembles with lattice spacings of about 0.15, 0.12, 0.09, and 0.06 fm, with the strange and charm quark masses near their physical values and the mass of the light quarks m_l set to $0.2m_s$. In the future, we plan to generate additional ensembles with lighter up and down quark masses. We present recent results on pion taste splittings, light hadron masses, the η_c dispersion relation and the topological susceptibility.

2. Implementation of the HISQ action

The HISQ action was developed to go beyond the asqtad action in its improvement of taste-symmetry. Links in the Dirac operator are replaced by

$$U' = \mathcal{F}_2 \mathcal{U} \mathcal{F}_1 U \quad (2.1)$$

where smearing level 1 denoted $\mathcal{F}_1$ is Fat 7; reunitarization is denoted by $\mathcal{U}$; and smearing level 2 denoted $\mathcal{F}_2$ is asq smearing.

To calculate the fermion force, we must take the derivative of the action with respect to the gauge link. With multilevel smearing, we must use the chain rule [5, 6]. For the fermion force, we have:

$$\frac{\partial S_f}{\partial U} = \frac{\partial S_f}{\partial X} \frac{\partial X}{\partial W} \frac{\partial W}{\partial V} \frac{\partial V}{\partial U}, \quad (2.2)$$

where U are the fundamental gauge links, V represent fat links after level 1 smearing, W are the result of reunitarizing V , and X are the links after asq smearing. Conveniently, code for three of the derivatives is the same as for the asqtad action (although the arguments may be different):

$$\frac{\partial S_f}{\partial X}, \frac{\partial X}{\partial W}, \frac{\partial V}{\partial U}. \quad (2.3)$$

After the first level of smearing, the link V must be projected into $U(3)$. This required some new code. We define: $W = VQ^{-1/2}$, with $Q = V^\dagger V$. The method to calculate the inverse square

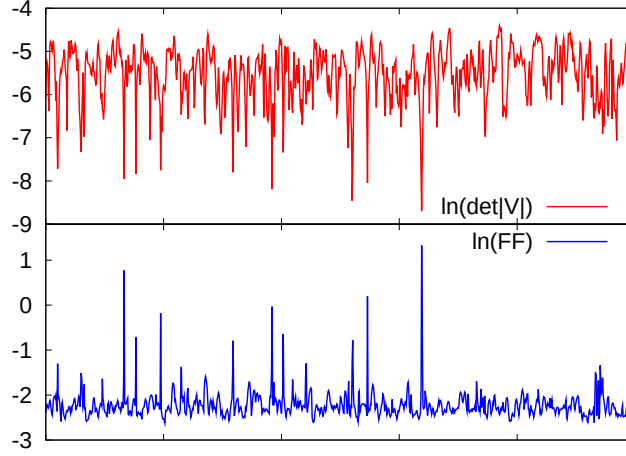


Figure 1: Time history of the minimum value of $\det|V|$ (upper plot) and the maximum magnitude of the fermion force (lower plot) [4]. Note how the large spikes in the fermion force are correlated with near vanishing of $\det|V|$. The lattice spacing is ≈ 0.13 fm.

root, based on the Cayley-Hamilton theorem, had already been applied by Morningstar & Peardon [7], and Hasenfratz, Hoffman & Shaefer [8].

$$Q^{-1/2} = f_0 + f_1 Q + f_2 Q^2. \quad (2.4)$$

We just need to find the eigenvalues of Q .

A significant issue in implementing molecular dynamics based on this algorithm is that there can be large changes in the action resulting from large forces during the integration of the equations of motion [4]. In Fig. 1, we see that there is a correlation between the large forces and low values of $\det|V|$. In Fig. 2, we show the fermion force rescaled by $1/\Delta t$ for runs with three different lattice spacings. (These two graphs are based on exploratory runs details of which can be found in Ref. [4].) It appears that as we approach the continuum, there are fewer large forces. As the fundamental links U are varying more smoothly, we should not be surprised that V is less likely to have a small determinant.

We implement an “eigenvalue filter” to tame the large forces. If the smallest eigenvalue of a smeared link V is smaller than a certain cutoff, we make the replacement $Q^{-1/2} \rightarrow (Q + \delta I)^{-1/2}$, where δ is typically set to 5×10^{-5} . Although this modifies the guiding Hamiltonian, the integration algorithm is still reversible and area preserving. As long as we use the RHMC algorithm [9], the accept/reject step at the end of each MD trajectory ensures the correct equilibrium distribution.

3. Testing the HISQ action

For our initial test of the HISQ action, we are generating ensembles with $m_l = 0.2m_s$ and lattice spacings varying from $a \approx 0.15$ to 0.06 fm. Table 1 shows the masses, lattice dimensions and acceptance rate on our tuning runs. In Table 2, we consider the production runs at the two intermediate lattice spacings. This range of lattice spacings is comparable to what we have with

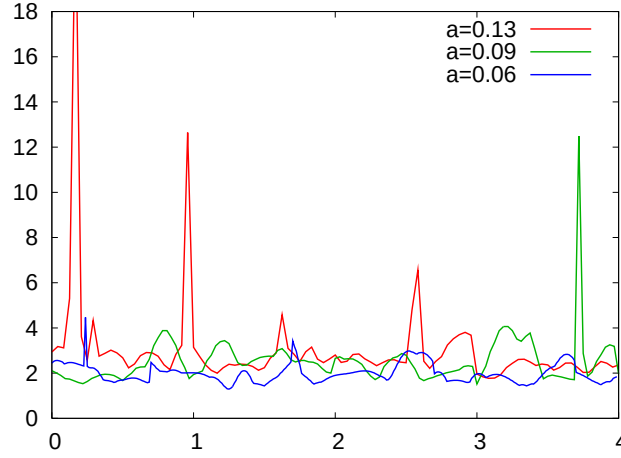


Figure 2: Time history of maximum value of the fermion force rescaled by the inverse time step for exploratory runs with three different lattice spacings. See Ref. [4] for run parameters.

β	am_l	am_s	am_c	size	a (fm)	acpt
5.80	0.0130	0.0650	0.838	$16^3 \times 48$	0.15	0.72
6.00	0.0102	0.0509	0.635	$20^3 \times 64$	0.12	0.68
6.30	0.0076	0.0380	0.445	$28^3 \times 96$	0.09	0.78
6.65	0.0054	0.0270	0.313	$48^3 \times 144$	0.06	0.70

Table 1: Parameters for tuning runs: coupling, dynamical quark masses in lattice units, lattice dimensions, approximate lattice spacing, and acceptance rate.

β	am_l	am_s	am_c	size	a (fm)	acpt
6.00	0.0102	0.0509	0.635	$24^3 \times 64$	0.12	0.74
6.30	0.0074	0.0370	0.440	$32^3 \times 96$	0.09	0.77

Table 2: Same as for Table 1, except for production runs.

the asqtad action [2] and we compare results for a number of quantities. We find that the pion taste splittings are reduced by a factor of 2.5 to 3, and that results with the HISQ action are comparable to those using the asqtad action at a lattice spacing of about 2/3 that used for the HISQ action.

4. Initial results

We present some initial results for the taste splittings of the pion, the spectrum of particles with light quarks, the η_c dispersion relation and the topological susceptibility. In most cases, the results are compared with prior work on asqtad configurations and it is found that the results with the HISQ action look closer to the continuum limit. (We do not have results for the η_c dispersion relation with asqtad quarks.)

4.1 Pion taste splittings

It is well known that for staggered quarks, taste symmetry breaking is an important lattice artifact. A prime motivation for HISQ quarks is to improve the taste symmetry. In Fig. 3, we compare the pion taste splittings for the asqtad [4] and HISQ actions. We see that for $a \approx 0.12$ fm, the taste splittings for the HISQ action are somewhat smaller than for asqtad with $a \approx 0.09$ fm. Similarly, results using the HISQ action with $a \approx 0.09$ fm are similar to results using the asqtad action with $a \approx 0.06$ fm. The vertical line to the left of this semi-log plot marked $\times 3$ is a ruler showing a factor of 3. We see that using the HISQ action reduces the taste splitting by a factor of 2.5 to 3 compared with asqtad.

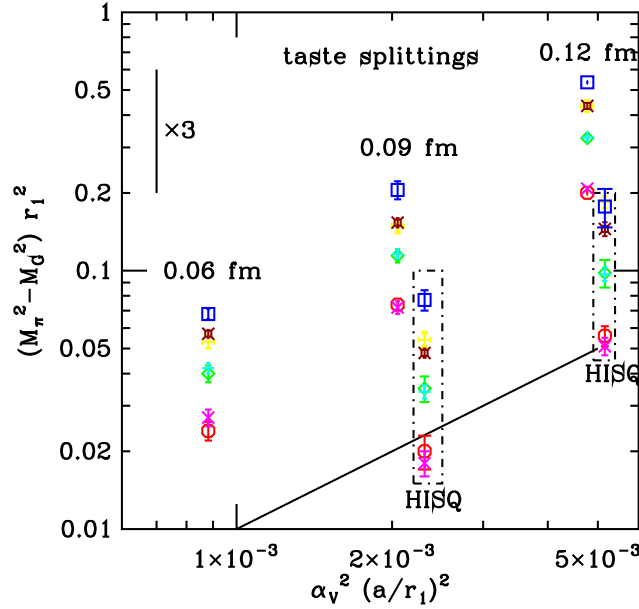


Figure 3: Calculation of taste splitting using the asqtad and HISQ actions. We show $(M_\pi^2 - M_G^2)r_1^2$ vs. $\alpha_v^2(a/r_1)^2$, where M_G is the Goldstone taste state. The diagonal line on this log-log plot shows the slope of the expected dependence of the taste splitting.

4.2 Spectrum of other light hadrons

We also have some preliminary results for the masses of ρ , nucleon and Ω^- . In each case, we find that using the HISQ action results in masses with smaller lattice spacing dependence, and the results are comparable to asqtad results at smaller lattice spacings. (The poster presented at the conference did not show results for ρ due to lack of space.) In Figs. 4 and 5, we show results for the ρ , nucleon and Ω^- . The improvement for the ρ seems quite substantial. For the nucleon, we find that the HISQ action result for $a \approx 0.15$ fm is quite a bit below the asqtad result with $a \approx 0.12$ fm. The HISQ result for $a \approx 0.09$ fm appears comparable to that for the asqtad action for $a \approx 0.06$ fm. The magenta curve represents a chiral perturbation theory fit to the asqtad results. For the Ω^- we also see a substantial improvement of HISQ action results over asqtad action results with $a \approx 0.12$ and 0.09 fm.

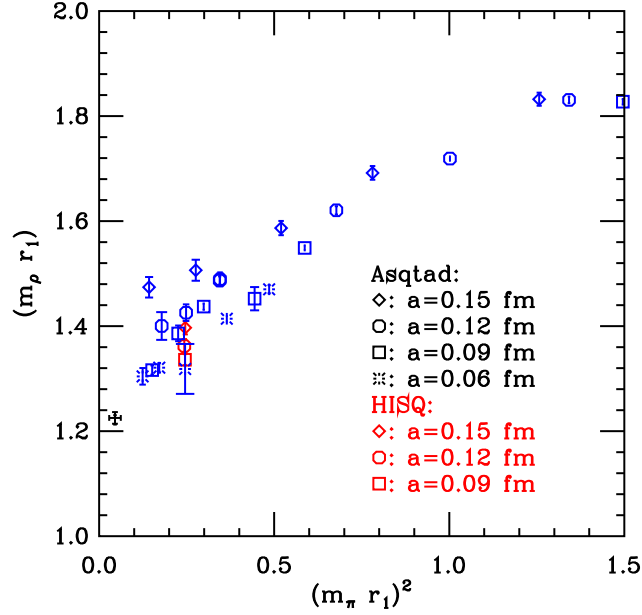


Figure 4: Rho mass in units of r_1 vs. the pion mass squared.

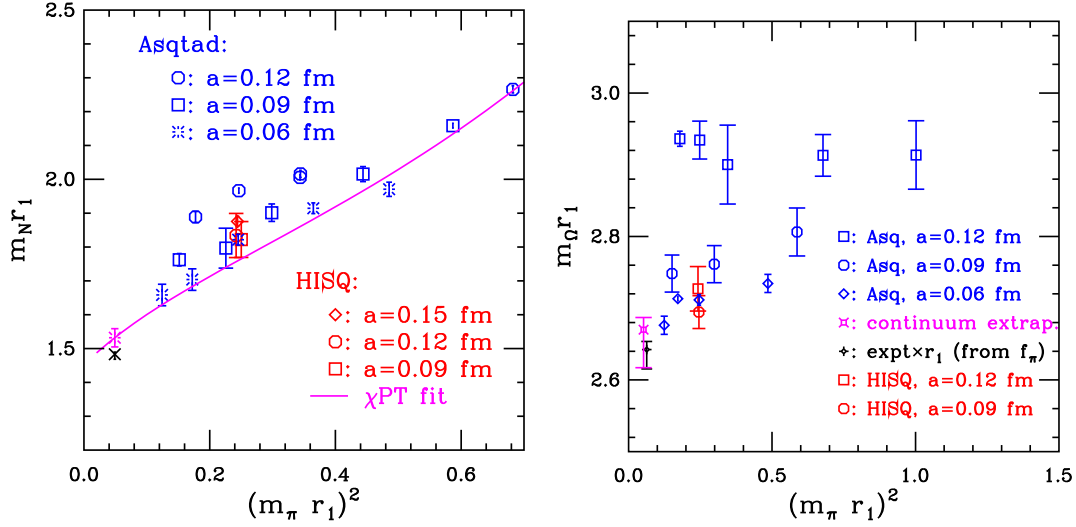


Figure 5: Nucleon mass (left) and Ω mass (right) in units of r_1 vs. the pion mass squared.

4.3 HISQ action and the charm quark

The HPQCD/UKQCD collaboration has developed a procedure for tuning the coefficient of the Naik term to reduce discretization errors up to $\mathcal{O}((am_c)^4)$. At tree level, the correction to the Naik term expressed in terms of the bare charm quark mass is [3]

$$\varepsilon = -\frac{27}{40}(am_c)^2 + \frac{327}{1120}(am_c)^4 - \frac{15607}{268800}(am_c)^6 - \frac{73697}{3942400}(am_c)^8. \quad (4.1)$$

Note that this formula differs from Eq. (24) in Ref. [3] because it is expressed in terms of the bare

mass appearing in the action. In Fig. 6, we show the dispersion relation for the η_c meson. For the three lattice spacings displayed, $-0.355 \leq \varepsilon \leq -0.123$. For $a \approx 0.06$ and $m_l = 0.2m_s$, $\varepsilon \approx -0.063$. We see that for a lattice spacing as coarse as 0.15 fm, the deviation from the continuum dispersion relation is as large as 7%; however, when the lattice spacing is reduced to 0.09 fm there is less than a 2% deviation from the continuum for the range of momentum shown here.

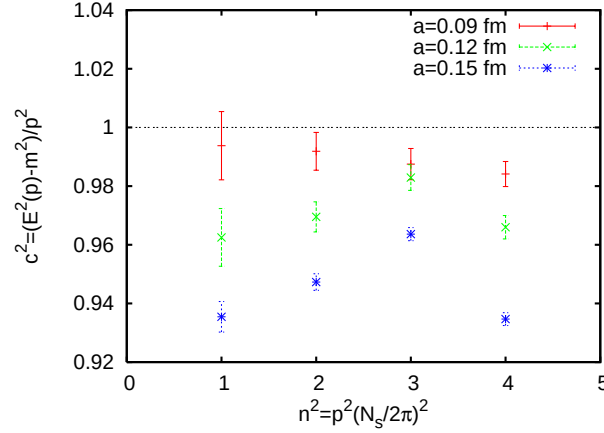


Figure 6: Speed of light from the η_c dispersion relation vs. lattice momentum squared.

4.4 Topological Susceptibility

In Fig. 7, we plot the topological susceptibility for both asqtad and HISQ action simulations. We find that the HISQ action point for $a \approx 0.12$ fm falls close to the asqtad action curve for $a \approx 0.09$ fm. Also note that the HISQ action point lies far to the left of the corresponding asqtad action $a \approx 0.12$ point (the third green square from the left) since the HISQ action taste symmetry is so much better than for the asqtad action, and the horizontal axis involves the taste singlet pion mass as shown by Billeter, DeTar and Osborn [10]. The black points and curve are from a continuum extrapolation of the fits to the results for the three asqtad lattice spacings.

5. Outlook

Based on the encouraging results of our preliminary scaling study with $m_l = 0.2m_s$, the MILC collaboration is planning to generate additional ensembles with $m_l = 0.1m_s$ and $0.04m_s$ for lattice spacings between 0.06 and 0.15 fm. These ensembles will allow us to study both the chiral and continuum limits. We expect to be able to study a wide variety of physics with these ensembles, for example, light pseudoscalar masses and decay constants, light quark spectroscopy, topology, spectroscopy of particles with a heavy quark, heavy-light meson decay constants and semileptonic decays, and quark masses.

Acknowledgements

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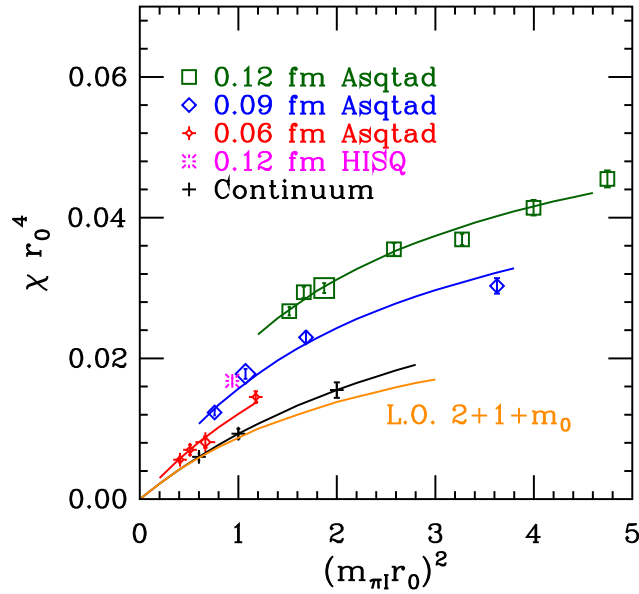


Figure 7: Topological susceptibility vs. squared mass of the taste singlet pion. The symbol size has been increased for the points coming from the asqtad action that correspond to $m_l = 0.2m_s$ so that they can more easily be compared with the HISQ action point. These points are either the second or third point from the left, depending on the lattice spacing.

References

- [1] The MILC collaboration: C. Bernard *et al.*, Nucl. Phys. (Proc. Suppl.), **60A** (1998) 297; Phys. Rev. D **58** (1998) 014503; G.P. Lepage, Nucl. Phys. (Proc. Suppl.), **60A** (1998) 267; Phys. Rev. D **59** (1999) 074501; K. Orginos and D. Toussaint (MILC), Nucl. Phys. (Proc. Suppl.), **73** (1999) 909; Phys. Rev. D **59** (1999) 014501; K. Orginos, D. Toussaint and R.L. Sugar (MILC), Phys. Rev. D **60** (1999) 054503; The MILC collaboration: C. Bernard *et al.*, Phys. Rev. D **61** (2000) 111502.
- [2] The MILC collaboration: A. Bazavov *et al.*, arXiv:0903.3598 [hep-lat], to appear in Reviews of Modern Physics.
- [3] E. Follana *et al.* [HPQCD collaboration and UKQCD collaboration], Phys. Rev. D **75** (2007) 054502 [arXiv:hep-lat/0610092].
- [4] The MILC collaboration: A. Bazavov *et al.*, PoS(LATTICE 2008)033 [arXiv:0903.0874 [hep-lat]].
- [5] W. Kamleh, D. B. Leinweber and A. G. Williams, Phys. Rev. D **70** (2004) 014502 [arXiv:hep-lat/0403019].
- [6] K. Y. Wong and R. M. Woloshyn, PoS(LATTICE2007)047 [arXiv:0710.0737 [hep-lat]].
- [7] C. Morningstar and M. J. Peardon, Phys. Rev. D **69** (2004) 054501 [arXiv:hep-lat/0311018].
- [8] A. Hasenfratz, R. Hoffmann and S. Schaefer, JHEP **0705** (2007) 029 [arXiv:hep-lat/0702028].
- [9] M. A. Clark and A. D. Kennedy, Phys. Rev. Lett. **98** (2007) 051601, [arXiv:hep-lat/0608015]; Phys. Rev. D **75** (2007) 011502 [arXiv:hep-lat/0610047].
- [10] B. Billeter, C. E. Detar and J. Osborn, Phys. Rev. D **70** (2004) 077502 [arXiv:hep-lat/0406032].

$B \rightarrow D^* l \nu$ at zero recoil: an update

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Fermilab Lattice and MILC Collaborations

We present an update of our calculation of the form factor for $\bar{B} \rightarrow D^* l \bar{\nu}$ at zero recoil, with higher statistics and finer lattices. As before, we use the Fermilab action for b and c quarks, the asqtad staggered action for light valence quarks, and the MILC ensembles for gluons and light quarks (Lüscher-Weisz married to 2+1 rooted staggered sea quarks). In this update, we have reduced the total uncertainty on $\mathcal{F}(1)$ from 2.6% to 1.7%.

At *Lattice2010* we presented a still-blinded result, but this writeup includes the unblinded result from the September 2010 CKM workshop.

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1. Introduction

The Wbc vertex is proportional to the coupling V_{cb} , which is an element of the Cabibbo [1] Kobayashi-Maskawa [2] (CKM) matrix. Along with the quark masses, it represents the observable part of the quarks' coupling to the Higgs sector and is, thus, a fundamental part of particle physics. The CKM matrix has four free parameters, and it is convenient to choose one of them to be (essentially) $|V_{cb}|$. Consequently, $|V_{cb}|$ appears throughout flavor physics [3].

$|V_{cb}|$ is determined from semileptonic decays $\bar{B} \rightarrow X_c l \bar{\nu}$, where X_c denotes a charmed final state. In *exclusive* decays, X_c is a D or D^* meson, and the decay amplitudes can be written

$$\langle D(v_D) | \gamma^\mu | \bar{B}(v_B) \rangle = \sqrt{M_B M_D} [(v_B + v_D)^\mu h_+(w) + (v_B - v_D)^\mu h_-(w)], \quad (1.1)$$

$$\langle D^*(v_D, \alpha) | \gamma^\mu | \bar{B}(v_B) \rangle = \sqrt{M_B M_{D^*}} \varepsilon^{\mu\nu}_{\rho\sigma} \bar{\varepsilon}_\nu^{(\alpha)} v_B^\rho v_{D^*}^\sigma h_V(w), \quad (1.2)$$

$$\langle D^*(v_D, \alpha) | \mathcal{A}^\mu | \bar{B}(v_B) \rangle = i\sqrt{M_B M_{D^*}} \bar{\varepsilon}_\nu^{(\alpha)} \{ g^{\nu\mu} (1+w) h_{A_1}(w) - v_B^\nu [v_B^\mu h_{A_2}(w) + v_{D^*}^\mu h_{A_3}(w)] \}, \quad (1.3)$$

where $\varepsilon^{(\alpha)}$ is the D^* polarization vector, v_B and $v_{D^{(*)}}$ denote the mesons' 4-velocities, and $w = v_B \cdot v_{D^{(*)}}$ is related to the invariant mass of the $l\bar{\nu}$ pair, $q^2 = M_B^2 + M_{D^{(*)}}^2 - 2wM_B M_{D^{(*)}}$. The form factors $h_\pm$, h_V , and h_{A_i} ($i = 1, 2, 3$) enjoy simple heavy-quark limits and are linear combinations of the form factors $f_\pm$, V , and A_i used in other semileptonic decays.

The differential decay distributions are

$$\frac{d\Gamma(\bar{B} \rightarrow D l \bar{\nu})}{dw} = \frac{G_F^2}{48\pi^3} m_D^3 (M_B + M_D)^2 (w^2 - 1)^{3/2} |V_{cb}|^2 |\mathcal{G}(w)|^2, \quad (1.4)$$

$$\frac{d\Gamma(\bar{B} \rightarrow D^* l \bar{\nu})}{dw} = \frac{G_F^2}{4\pi^3} m_{D^*}^3 (M_B - M_{D^*})^2 (w^2 - 1)^{1/2} |V_{cb}|^2 |\mathcal{F}(w)|^2, \quad (1.5)$$

neglecting the charged lepton and neutrino masses. The physical combinations of form factors are

$$\mathcal{G}(w) = h_+(w) - \frac{M_B - M_D}{M_B + M_D} h_-(w) = \frac{2\sqrt{M_B M_D}}{M_B + M_D} f_+(q^2), \quad (1.6)$$

$$\mathcal{F}(w) = h_{A_1}(w) \frac{1+w}{2} \sqrt{\frac{H_0^2(w) + H_+^2(w) + H_-^2(w)}{3\chi(w)}} \rightarrow h_{A_1}(1), \quad (1.7)$$

where the zero-recoil ($w \rightarrow 1$) limit of $\mathcal{F}$ is shown. The function $\chi(w)$ is chosen so that the square root in Eq. (1.7) collapses to 1 if $h_V = h_{A_3} = h_{A_1}$ and $h_{A_2} = 0$, as in the heavy-quark limit without radiative corrections. Expressions for $H_\pm(w)$, $H_0(w)$, and $\chi(w)$ can be found in Ref. [3].

The messy formula for $\mathcal{F}(w)$ indicates the advantage of the zero-recoil limit for $\bar{B} \rightarrow D^* l \bar{\nu}$: one must compute only $h_{A_1}(1)$, not four functions. In addition, the heavy-quark flavor symmetry is larger when $v_{D^*} = v_B$, and Luke's theorem applies. For determining $|V_{cb}|$, the key aspect of Luke's theorem is that it helps control systematic errors. In particular, in lattice gauge theories that respect heavy-quark symmetry, one can compute $h_{A_1}(1)$ with heavy-quark discretization errors that are formally $\bar{\Lambda}/m_Q$ times smaller than those of $h_{A_1}(w)$, $w \neq 1$, or those of $\mathcal{G}(w)$ even at $w = 1$.

Here we focus on $\bar{B} \rightarrow D^* l \bar{\nu}$ at zero recoil, describing our calculations of $\mathcal{F}(1) = h_{A_1}(1)$. Starting in 2001, experimental determinations of $|V_{cb}|$ used a quenched calculation [4]

$$\mathcal{F}(1) = 0.913_{-0.017}^{+0.024} \pm 0.016_{-0.014-0.016-0.014}^{+0.003+0.000+0.006}, \quad (1.8)$$

where the errors stem, respectively, from statistics, matching lattice gauge theory to QCD, lattice-spacing dependence, chiral extrapolation, and the quenched approximation. A notable feature of

Table 1: Parameters of the MILC ensembles used for heavy-quark physics. Here C denotes the number of configurations in each ensemble; (m'_l, m'_s) the asqtad sea-quark masses; m_q the asqtad valence masses; κ and c_{SW} the hopping parameter and clover coupling of the heavy quark. Standard nicknames for the lattice spacings are noted ($a \approx 0.045$ fm is “ultrafine”). Data are being generated on all ensembles for all m_q inside the $\{\dots\}$, but the present analysis uses at most two, namely $m_q = m'_l$ and $m_q = 0.4m'_s$.

a (fm)	Lattice	C	(am'_l, am'_s)	m_q	κ_b	κ_c	c_{SW}
≈ 0.15	$16^3 \times 48$	596	(0.0290, 0.0484)	{0.0484, 0.0453,			
medium	$16^3 \times 48$	640	(0.0194, 0.0484)	0.0421, 0.0290,			
coarse	$16^3 \times 48$	631	(0.0097, 0.0484)	0.0194, 0.0097,	0.0781	0.1218	1.570
	$20^3 \times 48$	603	(0.0048, 0.0484)	0.0068, 0.0048}			
≈ 0.12	$20^3 \times 64$	2052	(0.02, 0.05)	{0.05, 0.03,	0.0918	0.1259	1.525
coarse	$20^3 \times 64$	2259	(0.01, 0.05)	0.0415, 0.0349,	0.0901	0.1254	1.531
	$20^3 \times 64$	2110	(0.007, 0.05)	0.02, 0.01,	0.0901	0.1254	1.530
	$24^3 \times 64$	2099	(0.005, 0.05)	0.007, 0.005}	0.0901	0.1254	1.530
≈ 0.09	$28^3 \times 96$	1996	(0.0124, 0.031)	{0.031, 0.0261,	0.0982	0.1277	1.473
fine	$28^3 \times 96$	1946	(0.0062, 0.031)	0.0124,	0.0979	0.1276	1.476
	$32^3 \times 96$	983	(0.00465, 0.031)	0.0093, 0.0062,	0.0977	0.1275	1.476
	$40^3 \times 96$	1015	(0.0031, 0.031)	0.0047, 0.0031}	0.0976	0.1275	1.478
≈ 0.06	$48^3 \times 144$	668	(0.0072, 0.018)	{0.0188, 0.0160,	0.1052	0.1296	1.4276
superfine	$48^3 \times 144$	668	(0.0036, 0.018)	0.0072,	0.1052	0.1296	1.4287
	$56^3 \times 144$	800	(0.0025, 0.018)	0.0054, 0.0036,			
	$64^3 \times 144$	826	(0.0018, 0.018)	0.0025, 0.0018}			
≈ 0.045	$64^3 \times 192$	860	(0.0028, 0.014)	{0.014, 0.0056, 0.0028}			

Eq. (1.8) is that an estimate of the error associated with quenching has been made. Nevertheless, it is necessary to incorporate the light- and strange-quark sea. The first calculation with 2+1 flavors of sea quarks obtained [5]

$$\mathcal{F}(1) = 0.921 \pm 0.013 \pm 0.008 \pm 0.008 \pm 0.014 \pm 0.003 \pm 0.006 \pm 0.004, \quad (1.9)$$

where, now, the errors stem from statistics, the $g_{D^*D\pi}$ coupling, chiral extrapolation, discretization errors, matching, and two tuning errors. (The catch-phrases for the errors do not have exactly the same meaning in Refs. [4, 5]; for example, the $g_{D^*D\pi}$ error in Eq. (1.8) is incorporated into the chiral-extrapolation error.) This paper presents an update of the 2+1-flavor calculation, with mostly the same ingredients, but with higher statistics and without the second of the tuning errors.

The new data set is shown in Table 1, based as before on the MILC ensembles [6] with the Lüscher-Weisz gauge action [7], with the g^2N_c [8] but not g^2N_f corrections [9], and the asqtad-improved [10] rooted staggered determinant for the sea quarks. For the valence quarks, we use the asqtad action for the light quark and the Fermilab interpretation [11] of the clover action [12] for the heavy quark. In this report, we use all ensembles in Table 1 with entries for the heavy-quark couplings (κ_b , κ_c , and c_{SW}), *except* the fine $32^3 \times 96$ lattice. These data are being generated as part of a broad program of heavy-quark physics, including other semileptonic decays [13] and neutral-meson mixing and decay constants [14].

Improvements to $\mathcal{F}(1)$ are timely [3], because the values of $|V_{cb}|$ that follow from inclusive decays are in a 2.2σ tension with those that follow from Eq. (1.9) and also from $\bar{B} \rightarrow D l \bar{\nu}$ and $\mathcal{G}(1)$ [15]. The result described below is but one aspect of a resolution of the discrepancy. Others include a re-examination of the extrapolation to zero recoil, unquenched lattice-QCD calculations at $w \neq 1$, lattice-QCD calculations by other groups [16], and the incorporation of higher-order corrections to the inclusive decay expressions.

In Sec. 2, we discuss details of the data and of the data analysis. Because the value of $\mathcal{F}(1)$ has been studied so much in the past, any new analysis could be influenced in subtle human ways. To circumvent any such bias, we hide the numerical value of $\mathcal{F}(1)$ via an offset in the matching factor $\rho_{A^{cb}}$, explained in Sec. 3. We present our preliminary results, with all sources of uncertainty estimated, in Sec. 4. We include the unblinded value here, which was revealed after *Lattice 2010* but before these proceedings.

2. Data analysis

As in Ref. [5], we aim for the direct double-ratio

$$\mathcal{R}_{A_1} = \frac{\langle D^* | \bar{c} \gamma_j \gamma_5 b | \bar{B} \rangle \langle \bar{B} | \bar{b} \gamma_j \gamma_5 c | D^* \rangle}{\langle D^* | \bar{c} \gamma_4 c | D^* \rangle \langle B | b \gamma_4 b | B \rangle} = |h_{A_1}(1)|^2, \quad (2.1)$$

where the expressions here are all in (continuum) QCD. To this end, we use lattice gauge theory to compute the three-point correlation functions

$$C^{B \rightarrow D^*}(t_i, t_s, t_f) = \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \mathcal{O}_{D^*}(\mathbf{x}, t_f) \bar{\Psi}_c \gamma_j \gamma_5 \Psi_b(\mathbf{y}, t_s) \mathcal{O}_B^\dagger(\mathbf{0}, t_i) | 0 \rangle, \quad (2.2)$$

$$C^{B \rightarrow B}(t_i, t_s, t_f) = \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \mathcal{O}_B(\mathbf{x}, t_f) \bar{\Psi}_b \gamma_4 \Psi_b(\mathbf{y}, t_s) \mathcal{O}_B^\dagger(\mathbf{0}, t_i) | 0 \rangle, \quad (2.3)$$

$$C^{D^* \rightarrow D^*}(t_i, t_s, t_f) = \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \mathcal{O}_{D^*}(\mathbf{x}, t_f) \bar{\Psi}_c \gamma_4 \Psi_c(\mathbf{y}, t_s) \mathcal{O}_{D^*}^\dagger(\mathbf{0}, t_i) | 0 \rangle, \quad (2.4)$$

where $\mathcal{O}_B$ and $\mathcal{O}_{D^*}$ are interpolating operators coupling to the B and D^* mesons, and $\bar{\Psi}_c \gamma_\mu \Psi_b$ and $\bar{\Psi}_c \gamma_\mu \gamma_5 \Psi_b$ are improved currents [11, 4, 17, 5]. Then the lattice ratio

$$R_{A_1}(t) = \frac{C^{B \rightarrow D^*}(0, t, T) C^{D^* \rightarrow B}(0, t, T)}{C^{D^* \rightarrow D^*}(0, t, T) C^{B \rightarrow B}(0, t, T)} \quad (2.5)$$

should reach a plateau for a range of $t, T \gg t \gg 1$. The relationship between the plateau value of $R_{A_1}^{1/2}$ and $h_{A_1}(1)$ is discussed in Sec. 3.

With staggered fermions, $\mathcal{O}_B$ and $\mathcal{O}_{D^*}$ couple to both parities, and three-point correlation functions have four distinct contributions:

$$C^{X \rightarrow Y}(0, t, T) = \sum_{k=0} \sum_{\ell=0} (-1)^{kt} (-1)^{\ell(T-t)} A_{\ell k} e^{-M_X^{(k)} t} e^{-M_Y^{(\ell)} (T-t)} \quad (2.6)$$

$$\begin{aligned} &= A_{00}^{X \rightarrow Y} e^{-M_X t - M_Y (T-t)} + (-1)^{T-t} A_{01}^{X \rightarrow Y} e^{-M_X t - M_Y' (T-t)} + \\ &\quad (-1)^t A_{10}^{X \rightarrow Y} e^{-M_X' t - M_Y (T-t)} + (-1)^T A_{11}^{X \rightarrow Y} e^{-M_X' t - M_Y' (T-t)} + \dots \end{aligned} \quad (2.7)$$

with time-dependent factors of -1 associated with the states of undesired parity. To reduce the magnitude of the oscillating components, we form the combination [5]

$$\bar{R}_{A_1}(0, t, T) = \frac{1}{2}R_{A_1}(0, t, T) + \frac{1}{4}R_{A_1}(0, t, T+1) + \frac{1}{4}R_{A_1}(0, t+1, T+1), \quad (2.8)$$

which should tend more quickly to a plateau. The key here is to have $t_f = T$ and $T+1$.

The correlation functions and their ratios are analyzed for two light valence quark masses per ensemble, namely, $m_q = m'_l$ and $m_q = 0.4m'_s$ (or the single m_q when $m'_l = 0.4m'_s$). The choice of a fixed m_q , here $0.4m'_s$, for all m'_l matches, by design, our plans for the ultrafine lattice ($a \approx 0.045$ fm), to anchor future analyses even closer to the continuum limit. Typical plateaus are shown in Fig. 1 for a coarse, a fine, and a superfine ensemble. As one can see, the plateau in $\bar{R}_{A_1}$ emerges readily, and the statistical errors are 1% or smaller.

3. Matching, blinding, and discretization effects

The ratio combination $\bar{R}_{A_1}$ tends to a ratio of matrix elements like $\mathcal{R}_{A_1}$ in Eq. (2.1) but with lattice currents. Each current must be multiplied by a matching factor Z_A or Z_V , defined nonperturbatively in Ref. [17]. The lattice ratio R_{A_1} must, therefore, be multiplied by a matching ratio

$$\rho_{A^{\text{cb}}}^2 = Z_{A^{\text{cb}}}^2 / Z_V^{\text{cc}} Z_V^{\text{bb}}. \quad (3.1)$$

A subset of the collaboration has computed $\rho_{A^{\text{cb}}}$ in the one-loop approximation. The result is very close to unity, but the deviation is, or could be, comparable to $h_{A_1}(1) - 1$. Our numerical analysis replaces $\rho_{A^{\text{cb}}}$ with $F_{\text{blind}}\rho_{A^{\text{cb}}}$, where the *blinding factor* F_{blind} is again close to unity, but known only to those engaged in the one-loop calculation. In this way, choices of fitting ranges, etc., cannot be influenced by a human desire to (dis)agree with results for $\mathcal{F}(1)$ already in the literature.

The HQET-Symanzik formalism used to define the Z_J can also be used to control and suppress cutoff dependence [18, 17]. In the general case, several operators—both corrections to the current and insertions of the effective Lagrangian—generate cutoff effects. For details, see, *e.g.*, the discussion of Eq. (2.40) in Ref. [17]. For zero recoil, $v_{D^*} = v_B$, and the heavy-quark flavor symmetry enlarges from $U(1) \times U(1)$ to $SU(2)$. The leading discretization errors drop out, and the remainder can be found by applying the formulas of Ref. [18] to $\bar{R}_{A_1}^{1/2}$ and $h_{A_1}(1)$. One finds

$$\rho_{A^{\text{cb}}}\bar{R}_{A_1}^{1/2} = h_{A_1}(1) + O(\alpha_s a \Lambda^2 / m_c) + O(\alpha_s a^2 \Lambda^2) + O(\alpha_s^2), \quad (3.2)$$

where the last error acknowledges the one-loop calculation of $\rho_{A^{\text{cb}}}$. A study of the asymptotic

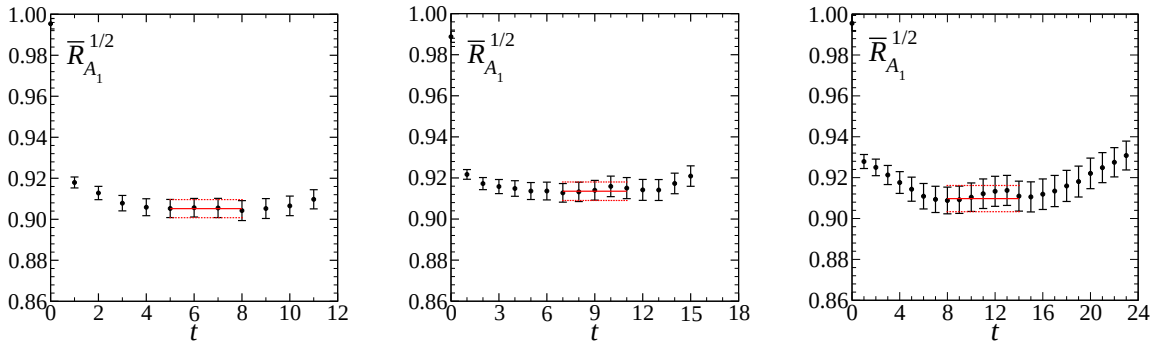


Figure 1: Ratio combination $\bar{R}_{A_1}^{1/2}(0, t, T)$ vs. t with $m_q = m'_l = 0.2m'_s$. From left to right: the coarse ensemble with $T = 12$ and $(am'_l, am'_s) = (0.01, 0.05)$; the fine ensemble with $T = 17$ and $(am'_l, am'_s) = (0.0062, 0.031)$; the superfine ensemble with $T = 24$ and $(am'_l, am'_s) = (0.0036, 0.018)$.

behavior of Fermilab actions provides a reasonable guide to the dependence on $m_Q a$ of the corrections. We see in our data little dependence on the lattice spacing, in accord with Eq. (3.2).

4. Preliminary result

Figure 2 provides a glimpse into our systematic error analysis, which closely follows Ref. [5]. We use our previous study of heavy-quark-mass dependence to fine-tune *a posteriori* the hopping parameters and to assess the tuning errors. We fit the light-quark mass dependence to one-loop chiral perturbation theory, suitably modified for staggered quarks [19]. The cusp is a necessary, physical effect that appears because the $D\pi$ threshold sinks below the D^* mass.

With the blinding factor in place, we find

$$F_{\text{blind}} \mathcal{F}(1) = 0.8949 \pm 0.0051 \pm 0.0088 \pm 0.0072 \pm 0.0093 \pm 0.0030 \pm 0.0050, \quad (4.1)$$

where the errors again stem from statistics, the $g_{D^* D \pi}$ coupling, chiral extrapolation, discretization errors, matching, and tuning κ_c and κ_b . To show how the errors have been reduced, it helps to scale this result to the old central value (F_F is the needed *ad hoc* factor):

$$\mathcal{F}(1) = 0.921(13)(8)(8)(14)(3)(6)(4) [5], \quad (4.2)$$

$$F_F \mathcal{F}(1) = 0.921(05)(9)(7)(10)(3)(5) \quad [\text{this work}]. \quad (4.3)$$

The higher statistics and wider scope of this dataset has reduced the statistical error with $C^{-1/2}$. The quoted heavy-quark discretization error is smaller, because with the superfine data we can move beyond pure power counting and combine the (lack of) trend in the data with the detailed theory of cutoff effects [18]. After Lattice 2010, we continued to examine the heavy-quark discretization and κ -tunings errors, reducing them somewhat, and the chiral-extrapolation error, increasing it somewhat. For the 2010 *Workshop on the CKM Unitarity Triangle*, we removed the blinding factor, finding [20]:

$$\mathcal{F}(1) = 0.9077(51)(88)(84)(90)(30)(33). \quad (4.4)$$

This result reduces the tension with $|V_{cb}|$ from inclusive decays to 1.6σ .

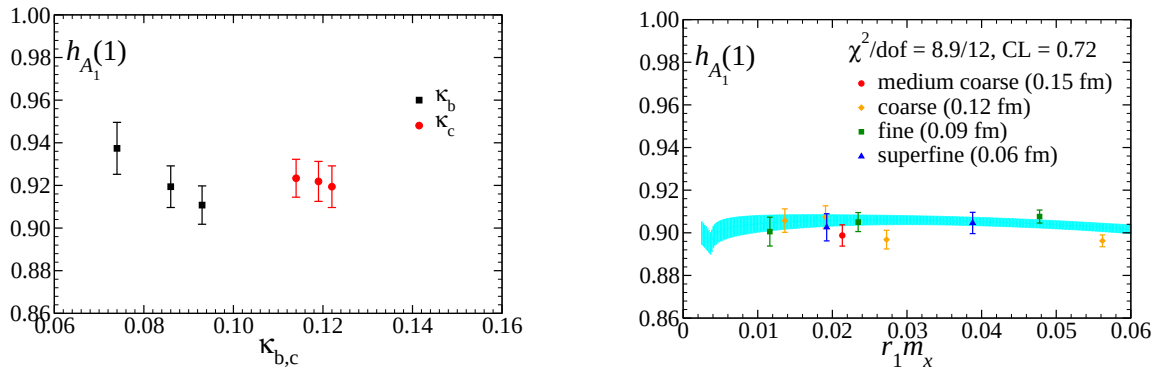


Figure 2: Left: dependence of $h_{A_1}(1)$ on the heavy-quark hopping parameters (with data of Ref. [5]). Right: chiral extrapolation showing only points with $m_q = m_l$ and a fit to all data.

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References

- [1] N. Cabibbo, *Phys. Rev. Lett.* **10** (1963) 531.
- [2] M. Kobayashi and T. Maskawa, *Prog. Theor. Phys.* **49** (1973) 652.
- [3] M. Antonelli *et al.*, *Phys. Rept.* **494** (2010) 197 [arXiv:0907.5386 [hep-ph]].
- [4] S. Hashimoto, A.S. Kronfeld, P.B. Mackenzie, S.M. Ryan, and J.N. Simone, *Phys. Rev. D* **66** (2002) 014503 [arXiv:hep-ph/0110253].
- [5] C. Bernard *et al.* [Fermilab Lattice and MILC Collaborations], *Phys. Rev. D* **79** (2009) 014506 [arXiv:0808.2519 [hep-lat]].
- [6] A. Bazavov *et al.*, *Rev. Mod. Phys.* **82** (2010) 1349 [arXiv:0903.3598 [hep-lat]].
- [7] M. Lüscher and P. Weisz, *Commun. Math. Phys.* **97** (1985) 59 [Erratum *ibid.* **98** (1985) 433].
- [8] M. Lüscher and P. Weisz, *Phys. Lett. B* **158** (1985) 250.
- [9] Z. Hao, G.M. von Hippel, R.R. Horgan, Q.J. Mason, and H.D. Trotter, *Phys. Rev. D* **76** (2007) 034507 [arXiv:0705.4660 [hep-lat]].
- [10] G.P. Lepage, *Phys. Rev. D* **59** (1999) 074502 [hep-lat/9809157].
- [11] A.X. El-Khadra, A.S. Kronfeld, and P.B. Mackenzie, *Phys. Rev. D* **55** (1997) 3933 [arXiv:hep-lat/9604004].
- [12] B. Sheikholeslami and R. Wohlert, *Nucl. Phys. B* **259** (1985) 572.
- [13] J.A. Bailey *et al.* [Fermilab Lattice and MILC Collaborations], *PoS(Lattice 2010)* 306.
- [14] C.M. Bouchard *et al.* [Fermilab Lattice and MILC Collaborations], *PoS(Lattice 2010)* 299.
- [15] M. Okamoto *et al.* [Fermilab Lattice and MILC Collaborations], *Nucl. Phys. Proc. Suppl.* **140** (2005) 461 [arXiv:hep-lat/0409116].
- [16] G.M. de Divitiis, E. Molinaro, R. Petronzio, and N. Tantalo, *Phys. Lett. B* **655** (2007) 45 [arXiv:0707.0582 [hep-lat]]; G.M. de Divitiis, R. Petronzio, and N. Tantalo, *Nucl. Phys. B* **807** (2009) 373 [arXiv:0807.2944 [hep-lat]].
- [17] J. Harada, S. Hashimoto, A.S. Kronfeld, and T. Onogi, *Phys. Rev. D* **65** (2002) 094514 [arXiv:hep-lat/0112045].
- [18] A.S. Kronfeld, *Phys. Rev. D* **62** (2000) 014505 [arXiv:hep-lat/0002008].
- [19] J. Laiho and R. S. Van de Water, *Phys. Rev. D* **73** (2006) 054501 [arXiv:hep-lat/0512007].
- [20] P.B. Mackenzie, talk at *Workshop on the CKM Unitarity Triangle*, Warwick, UK (September 2010).

B_s^0 and B^0 Mixing in the Standard Model and Beyond: A Progress Report

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We give a progress report on the calculation of B meson mixing matrix elements, focusing on contributions that could arise beyond the Standard Model. The calculation uses asqtad (light quark) and Fermilab (heavy quark) valence actions and MILC ensembles with 2+1 flavors of asqtad sea quarks. We report preliminary B_s^0 fit results, at a lattice spacing of 0.12 fm, for the SUSY basis of effective four-quark mixing operators and include an estimate for the final error budget.

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1. Introduction

1.1 Motivation

The absence of tree-level flavor-changing neutral currents in the SM means its contributions to neutral meson mixing begin at the loop level. The B_s^0 (B^0) mixing amplitude is further suppressed by a combination of the GIM mechanism and the CKM matrix element $|V_{ts}|^2 \sim 2 \times 10^{-3}$ ($|V_{td}|^2 \sim 6 \times 10^{-5}$), opening the door for observable new physics effects [1].

A number of recent analyses have revealed hints of new physics in B_s^0 and B^0 mixing. A $(2-3)\sigma$ tension in the Unitarity Triangle can be explained by new physics in $\Delta M_s/\Delta M_d$ [2]. The UTfit collaboration performed a simultaneous analysis of multiple experimental results, finding $\sim 3\sigma$ evidence of new physics in B_s^0 mixing [3]. $D0$'s recent report of an anomalous like-sign dimuon charge asymmetry in semileptonic b-hadron decay deviates from the SM prediction by $\sim 3\sigma$, providing additional evidence of new physics in B_s^0 mixing [4, 5].

Disagreement between SM mixing predictions and experiment motivates increased precision in the calculation of SM hadronic mixing matrix elements. These calculations have been performed on the lattice, with $2+1$ dynamical sea quarks, to a $(3-4)\%$ precision [6, 7], but further refinements are needed to sort out tension with experiment. To permit mixing predictions from new physics models, a knowledge of the possible BSM hadronic mixing matrix elements is required. Pioneering work [8, 9], utilizing the quenched approximation and static limit of HQET, resulted in a quoted $\sim 10\%$ precision. We aim to improve upon this.

1.2 The Role of Lattice QCD

Whether considering SM or beyond, the disparate scales of hadronization, $\mathcal{O}(500 \text{ MeV})$, and the underlying flavor-changing physics¹ results in a factorization of the physics at the two scales. For example, the SM expression for the oscillation frequency of the $B_q^0 \leftrightarrow \overline{B}_q^0$ transition [10],

$$(\Delta M_q)_{SM} = \left(\frac{G_F^2 M_W^2 S_0}{4\pi^2 M_{B_q}} \right) \eta_B(\mu) |V_{tb}V_{tq}^*|^2 \langle B_q^0 | O(\mu) | \overline{B}_q^0 \rangle, \quad (1.1)$$

separates the low energy physics of hadronization, characterized by the mixing hadronic matrix element $\langle B_q^0 | O | \overline{B}_q^0 \rangle$, from the details of the flavor-changing interactions of the SM. The SM plays a role in $\langle B_q^0 | O | \overline{B}_q^0 \rangle$ by restricting the structure of the effective four-quark operator O . For a generic underlying theory we can write

$$\Delta M_q = \sum_i c_i(\mu) \langle B_q^0 | O_i(\mu) | \overline{B}_q^0 \rangle, \quad (1.2)$$

where the short distance Wilson coefficients, c_i , contain the details of the underlying theory and are generally perturbatively calculable. The O_i are all effective, four-quark, $\Delta B = 2$ (B is the bottom quark flavor quantum number) operators allowed by the theory.

Lattice QCD permits calculation of the non-perturbative, purely hadronic quantities $\langle B_q^0 | O_i | \overline{B}_q^0 \rangle$.

¹In the SM this is the electroweak scale, $\mathcal{O}(100 \text{ GeV})$, and in new physics models is typically larger.

2. Calculation

2.1 Generating Data

The space of possible Lorentz-invariant, color singlet, four-quark mixing operators is spanned by a basis of mixing operators, referred to for historical reasons as the SUSY basis [11],

$$\begin{aligned} O_1 &= (\bar{b}^\alpha \gamma_\mu P_L q^\alpha) (\bar{b}^\beta \gamma_\mu P_L q^\beta), & O_2 &= (\bar{b}^\alpha P_L q^\alpha) (\bar{b}^\beta P_L q^\beta), \\ O_3 &= (\bar{b}^\alpha P_L q^\beta) (\bar{b}^\beta P_L q^\alpha), & O_4 &= (\bar{b}^\alpha P_L q^\alpha) (\bar{b}^\beta P_R q^\beta), \text{ and} \\ O_5 &= (\bar{b}^\alpha P_L q^\beta) (\bar{b}^\beta P_R q^\alpha), \end{aligned} \quad (2.1)$$

listed here with greek color and suppressed spin indices. Of 20 potential mixing operators, 12 can be eliminated by Fierz transformation and three by parity symmetry of QCD. We're studying the possibility of using these extra operators to effectively increase statistics. For each O_N we write the mixing three-point correlation function as a time-ordered VEV of interpolating and mixing operators (a similar, if simpler, process is used to construct two-point correlation functions):

$$C_N^{3pt}(t_1, t_1) = \sum_{\vec{x}_1, \vec{x}_2} \langle T \{ (\bar{q} \gamma_5 b)_{\vec{x}_2, t_2} (O_N)_{\vec{0}, 0} (\bar{q} \gamma_5 b)_{\vec{x}_1, t_1} \} \rangle, \quad (2.2)$$

$$C_{PS}^{2pt}(t) = \sum_{\vec{x}} \langle T \{ (\bar{q} \gamma_5 b)_{\vec{x}, t} (q \gamma_5 \bar{b})_{\vec{0}, 0} \} \rangle. \quad (2.3)$$

Wick contraction yields products of quark propagators with time ordering ensured by imposing $t_2 > 0 > t_1$ and $t > 0$. Heavy (light) quark propagators are obtained by inverting the Fermilab (asqtad) action on MILC gauge configurations with $2 + 1$ dynamical asqtad sea quarks [12]. A summary of gauge field configurations used (or planned for use) is given in Table 1. We work in the meson rest frame by Fourier transforming the correlation functions and setting $\vec{p} = 0$, leaving

$\approx a$ (fm)	$L^3 \times T$	β	m_l/m_s	$m_\pi L$	$N_c \times N_t$
0.12	$24^3 \times 64$	6.760	0.1	3.84	2099×4
0.12	$20^3 \times 64$	6.760	0.14	3.78	2110×4
0.12	$20^3 \times 64$	6.760	0.2	4.48	2259×4
0.12	$20^3 \times 64$	6.790	0.4	6.22	2052×4
0.09	$40^3 \times 96$	7.080	0.1	4.21	1015×4
0.09	$32^3 \times 96$	7.085	0.15	4.11	984×4
0.09	$28^3 \times 96$	7.090	0.2	4.14	1931×4
0.09	$28^3 \times 96$	7.110	0.4	5.78	1996×4
0.06	$64^3 \times 144$	7.460	0.1	4.27	$826 \times N_t$
0.06	$56^3 \times 144$	7.465	0.14	4.39	$800 \times N_t$
0.06	$48^3 \times 144$	7.470	0.2	4.49	$668 \times N_t$
0.06	$48^3 \times 144$	7.480	0.4	6.33	$668 \times N_t$
0.045	$64^3 \times 192$	7.810	0.2	4.56	$860 \times N_t$

Table 1: MILC ensembles [12] planned for use in this study. $N_c \times N_t$ is the number of configurations and source times (not yet determined if unspecified). This report includes results for the $a = 0.12$ fm ensembles.

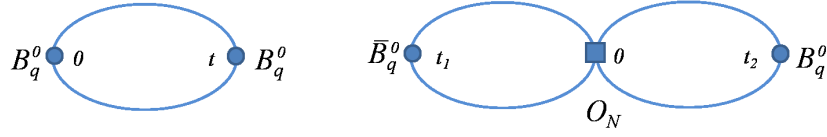


Figure 1: (left) Two- and (right) three-point correlation functions in the meson rest frame. The mixing operator is placed at the origin in the three-point correlation function.

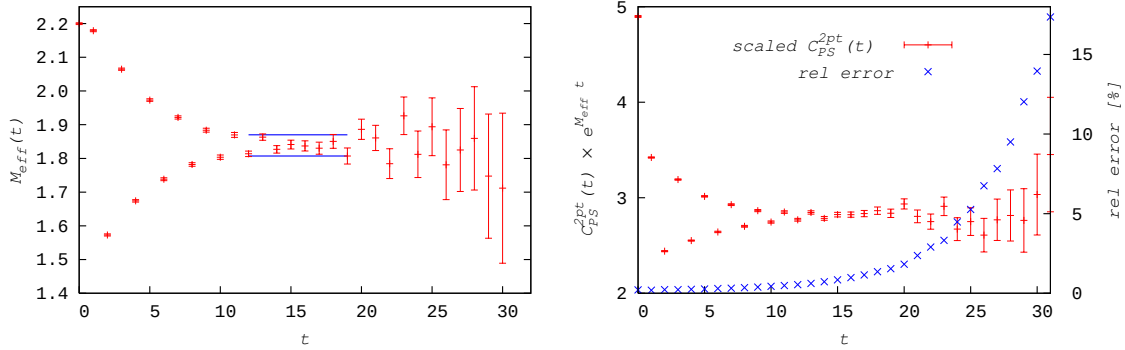


Figure 2: (left) B_s effective mass plot and (right) scaled two-point pseudo-scalar correlation function on the $a = 0.12$ fm, 20×64^3 , $m_l/m_s = 0.4$ ensemble. Source and sink are 1S-smeared.

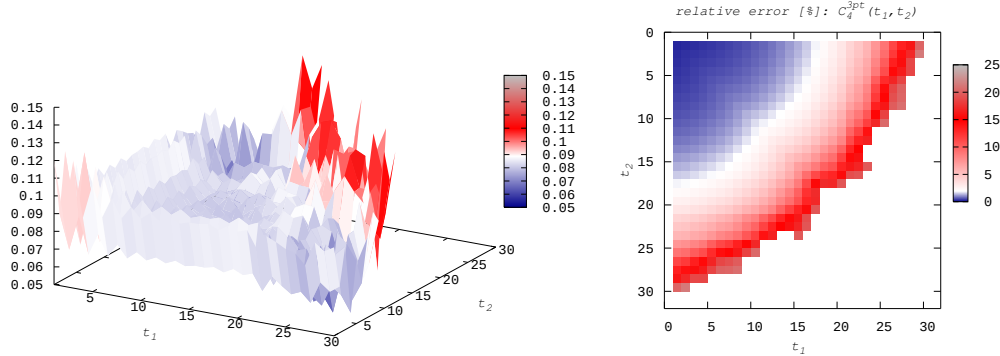


Figure 3: (left) The scaled B_s three-point correlation function for mixing operator $O_4 = (\bar{b}^\alpha L q^\alpha) (\bar{b}^\beta R q^\beta)$ and (right) its relative error on the $a = 0.12$ fm, 20×64^3 , $m_l/m_s = 0.4$ ensemble. The heavy quark fields are 1S-smeared at the sinks.

correlation functions that depend only on time (depicted in Fig. 1). In the three-point correlation functions, the heavy quark fields in the mixing operator are improved to remove a discretization error [13] and 1S-smeared at the sinks to increase ground state overlap. Heavy quark fields in the two-point correlation functions are 1S-smeared at the source and sink. Figs. 2 and 3 show plots of two- and three-point correlation function data generated in this way. All data and fit results shown are for the B_s meson ($\kappa = 0.0918$ and $ma = 0.0349$).

2.2 Fitting

We build fit functions by decomposing the two- and three-point correlation functions of Eqs. (2.2

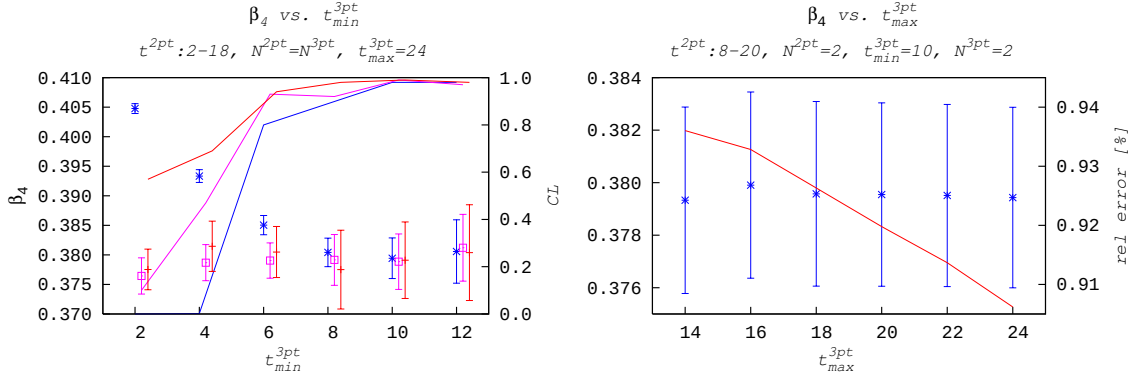


Figure 4: Simultaneous fits of C_{PS}^{2pt} and C_4^{3pt} on the $a = 0.12$ fm, 20×64^3 , $m_l/m_s = 0.4$ ensemble for the B_s mixing parameter β_4 , defined in Sect. 3. (left) Fits vs. $t_{\min}$ (shown for $t_{\max} = 24$) reveal a common plateau for $N^{3pt} = N^{2pt} = 2$ (blue burst), 4 (pink square) and 6 (red dash) fits. Solid lines indicate confidence levels for the fits. (right) We plot a representative fit from the plateau ($N^{3pt} = 2$ and $t_{\min}^{3pt} = 10$) to demonstrate stability with respect to $t_{\max}^{3pt}$. Fits are blue bursts with error bars and the solid red line is the relative error.

and 2.3) in a basis of energy eigenstates, giving an infinite sum of exponentials

$$C_{PS}^{2pt}(t) = \sum_{n=0}^{\infty} \frac{|Z_n|^2}{2E_n} (-)^{n(t+1)} \left(e^{-E_n t} + e^{-E_n(T-t)} \right) \quad (2.4)$$

$$C_N^{3pt}(t_1, t_1) = \sum_{n,m=0}^{\infty} \frac{\langle n | O_N | m \rangle Z_n^\dagger Z_m}{4E_n E_m} (-)^{n(t_1+1)+m(t_2+1)} \left(e^{-E_n |t_1|} + e^{-E_n(T-|t_1|)} \right) \left(e^{-E_m t_2} + e^{-E_m(T-t_2)} \right)$$

where $Z_n \equiv \langle n | \bar{q} \gamma_5 b \rangle$. Oscillating opposite parity states, a result of staggered light valence quarks [14], and the effect of periodic boundary conditions are accounted for in Eq. (2.4). In practice, we limit the time range of data included in the fit ($t_{\min} \leq t \leq t_{\max}$) and truncate the sums ($\sum_{n=0}^{N^{2pt}-1}$ and $\sum_{n,m=0}^{N^{3pt}-1}$), where $N^{2,3pt}$ is the number of states used in the fit.

Fits using data at short times must account for increased excited state contributions by including an adequate number of states. Despite added difficulty, the relatively clean signal in the data at short times may make it desirable to include them in the fit. We accomplish this using a Bayesian fitting routine [15, 16] and a systematic procedure to select N , $t_{\min}$ and $t_{\max}$. We are able to achieve consistent and stable fits, with a suitable choice of time range, for $N^{2,3pt} = 2, 4$ and 6.

From scaled correlation functions we determine time ranges to study. For $t_{\min}$ we generally consider from $t_{\min} = 2$ until excited state contributions have significantly decreased. Though increasing $t_{\max}$ utilizes more data, it also introduces an increasing level of noise and can lead to an underdetermined covariance matrix. For the two-point correlation function of Fig. 2 we considered $t_{\min}^{2pt} = 2, 4, \dots, 12$ and $t_{\max}^{2pt} = 12, 14, \dots, 24$, for the three-point correlation function of Fig. 3, $t_{\min}^{3pt} = 2, 4, \dots, 12$ and $t_{\max}^{3pt} = 14, 16, \dots, 24$, and in each case $N^{2,3pt} = 2, 4, 6$.

We fit for each combination of N^{2pt} , $t_{\min}^{2pt}$ and $t_{\max}^{2pt}$ and select a representative fit from the common plateau, ensuring stability with respect to our choice of N^{2pt} , $t_{\min}^{2pt}$ and $t_{\max}^{2pt}$. Then, fixing the two-point fit parameters, we repeat the procedure for a simultaneous fit of the two- and three-point correlation functions. Fig. 4 demonstrates the stability of the simultaneous fits.

2.3 Initial Results

Table 2 lists preliminary fit results for the B_s mixing parameters, β_N , defined by $\langle B_q^0 | O_N | \overline{B}_q^0 \rangle = \mathcal{C}_N M_{B_q} \beta_N^2$ ($\mathcal{C}_1 = 2/3$, $\mathcal{C}_2 = -5/12$, $\mathcal{C}_3 = 1/12$, $\mathcal{C}_4 = 1/2$, and $\mathcal{C}_5 = 1/6$).

$m_l/m_s =$	0.4	0.2	0.14	0.1
$\beta_1 \times (r_1/a)^{3/2} =$	1.217(14)	1.196(11)	1.160(14)	1.161(14)
$\beta_2 \times (r_1/a)^{3/2} =$	1.509(15)	1.446(14)	1.425(16)	1.448(14)
$\beta_3 \times (r_1/a)^{3/2} =$	1.490(22)	1.409(25)	1.318(34)	1.446(25)
$\beta_4 \times (r_1/a)^{3/2} =$	1.785(14)	1.731(12)	1.689(14)	1.699(13)
$\beta_5 \times (r_1/a)^{3/2} =$	2.313(26)	2.255(14)	2.200(21)	2.223(13)

Table 2: Preliminary fit results for β_N on the $a = 0.12$ fm ensembles. Errors are statistical from the fit.

3. Outlook

We are extending B_s^0 fits to other lattice spacings and a range of valence masses, to include B_d^0 . We will use these fits in an extrapolation to physical light sea quark mass, the continuum, and light valence quark mass (and an interpolation to physical strange quark mass). The continuum [17] and staggered lattice [18] chiral perturbation theory has been worked out. One-loop perturbative renormalization for the SM mixing operators exists and the BSM operator renormalization is expected to be a simple extension of this work.

Source of Error [%]	β_1 (<i>Lattice 2009</i>)	Expected	Reference
statistical	2.7	1.2	current work
scale (r_1)	3.0	1.0	[19]
sea & valence quark masses	0.3	0.3	
b-quark hopping parameter	≤ 0.5	0.1	[20]
χ PT + light quark discretization	0.4	< 0.4	*
$\mathcal{G}_{B^*B\pi}$	0.3	< 0.3	*
heavy quark discretization	2	~ 1.2	[20]
matching (1-loop perturbation theory)	~ 4	~ 2.5	[21]
finite volume effects	≤ 0.5	< 0.1	[20]
Total	6.1	~ 3.2	

Table 3: We estimate an error budget, for β_1 , by way of comparison with [7]. The sources of expected improvements are listed in the Reference column. *We anticipate improvement from finer lattice spacings.

Accurately accounting for errors in the calculation is as important as achieving precision results. Our naive statistical errors represent a (40-50)% reduction relative to [7]. We are generating more robust estimates via the bootstrap method. Correlator data exist for $a = 0.12, 0.09$ fm and

are being generated for $a = 0.06, 0.045$ fm. Table 3 quotes statistical and systematic errors for β_1 from [7], with expected improvements from the use of $a = 0.06$ fm data. Analysis of $a = 0.045$ fm data will further improve the error budget.

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References

- [1] A. Buras, PoS EPS-HEP2009: 024 (2009) [arXiv:0910.1032 [hep-ph]].
- [2] E. Lunghi and A. Soni, Phys. Lett. B **666**: 162-165 (2008) [arXiv:0803.4340 [hep-ph]]; J. Laiho, E. Lunghi, and R.S. Van de Water, Phys. Rev. D **81**: 034503 (2010) [arXiv:0910.2928 [hep-ph]]; A. Lenz *et al.*, arXiv:1008.1593 [hep-ph].
- [3] M. Bona *et al.* (UTfit Collaboration), PMC Phys. A3: 6 (2009) [arXiv:0803.0659 [hep-ph]].
- [4] V.M. Abazov *et al.* (D0 Collaboration), Phys. Rev. D **82**: 032001 (2010) [arXiv:1005.2757 [hep-ex]].
- [5] A. Lenz and U. Nierste, JHEP **0706**: 072 (2007) [arXiv:hep-ph/0612167].
- [6] E. Gámiz *et al.* (HPQCD Collaboration), Phys. Rev. D **80**: 014503 (2009) [arXiv:0902.1815 [hep-lat]]; O. Witzel *et al.*, PoS LAT2009: 243 (2009).
- [7] R. Todd Evans *et al.*, PoS LAT2009: 245 (2009).
- [8] V. Giménez and J. Reyes, Nucl. Phys. Proc. Suppl. **94**: 350-353 (2001) [arXiv:hep-lat/0010048].
- [9] D. Becirevic *et al.*, JHEP 0204 (2002) 025 [arXiv:hep-lat/0110091].
- [10] A.J. Buras, M. Jamin, and P.H. Weisz, Nucl. Phys. B **347**: 491 (1990).
- [11] F. Gabbiani, E. Gabrielli, A. Masiero, and L. Silvestrini, Nucl. Phys. B **477**: 321-352 (1996) [arXiv:hep-ph/9604387].
- [12] A. Bazavov *et al.* (MILC Collaboration), Rev. Mod. Phys. **82**: 1349-1417 (2010) [arXiv:0903.3598 [hep-lat]].
- [13] A. El-Khadra, A. Kronfeld, and P.B. Mackenzie, Phys. Rev. D **55**: 3933 (1997) [arXiv:hep-lat/9604004].
- [14] M. Wingate, J. Shigemitsu, C.T. Davies, G.P. Lepage, and H. Trotter, Phys. Rev. D **67**: 054505 (2003) [arXiv:hep-lat/0211014].
- [15] G.P. Lepage *et al.*, arXiv:hep-lat/0110175 (2001).
- [16] G.P. Lepage's Python-based library for Bayesian least squares fitting of multi-dimensional, nonlinear functions of arbitrarily many parameters, built around `lsqfit` (2008).
- [17] W. Detmold and C.-J. David Lin, Phys. Rev. D **76**: 014501 (2007) [arXiv:hep-lat/0612028].
- [18] J. Laiho and R.S. Van de Water, Collaboration Note (2007).
- [19] A. Bazavov *et al.* (MILC Collaboration), PoS LAT2009: 079 (2009).
- [20] R.T. Evans *et al.* (Fermilab Lattice and MILC Collaborations), *in preparation*.
- [21] Estimate based on using $a = 0.06$ fm ensembles.

Numerical Tests of the Improved Fermilab Action

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Recently, the Fermilab heavy-quark action was extended to include dimension-six and -seven operators in order to reduce the discretization errors. In this talk, we present results of the first numerical simulations with this action (the OK action), where we study the masses of the quarkonium and heavy-light systems. We calculate combinations of masses designed to test improvement and compare results obtained with the OK action to their counterparts obtained with the clover action. Our preliminary results show a clear improvement.

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1. Introduction

Simulating heavy quarks in lattice QCD is a challenging problem, because the quark mass m_Q and the accessible ultraviolet cutoff a^{-1} are comparable. Special care is needed to handle discretization errors [1]. In order to make accurate and reliable calculations of many Standard Model parameters involving heavy quarks, one needs not only computer power but also methodological improvements of the quark actions used. One line of attack is the Fermilab method [2], which starts with the clover action [3] for Wilson fermions [4]. In the original work, interactions through dimension five were considered. More recently, we extended the Fermilab method to an action (the OK action) with dimension-six and -seven interactions [5, 6].

Using power counting as a guide, Ref. [5] estimated that the OK action should reduce discretization effects for heavy quarks to $\sim 1\%$ on, say, the MILC asqtad ensembles [7]. In this paper, we present the first numerical results obtained with the OK action, to test whether the theoretical improvement is realized in practice. We compute combinations of rest masses and kinetic masses designed to test the improvement, without the need to tune the input parameters.

In Sec. 2, we briefly discuss and present the OK action. Section 3 contains the details of the simulations and our preliminary results for an inconsistency I [8], and for the hyperfine splittings between rest and kinetic masses for the heavy-heavy and heavy-light systems. We discuss our results and future plans in section 4.

2. OK Action and Tadpole Improvement

In this section, we briefly describe the OK action, including the tadpole improvement [9] used in the simulation. In general, the Fermilab formalism calls for separate couplings for spatial and temporal interactions. Fermilab actions have a smooth transition to the $m_0 a \rightarrow 0$ and $m_0 a \rightarrow \infty$ limits, but the short-distance coefficients depend on $m_0 a$, ζ and the spatial Wilson parameter r_s in a non-trivial way [2]. This action reduces the discretization errors to $O(a^2 \Lambda^2 b(m_Q a))$, where b is a function that is bounded for all $m_Q a$. The OK action includes higher dimensional operators to further reduce the lattice spacing errors.

Reference [5] starts by considering all the operators of dimension six and seven with two effective field theories in mind: heavy-quark effective theory (HQET) and the nonrelativistic QCD (NRQCD), appropriate to heavy-light and heavy-heavy systems, respectively. The interactions are classified in powers of λ (HQET, $\lambda \sim \Lambda/m_Q$, Λa) or v (NRQCD, relative internal velocity). Once all the independent operators are identified, the redundant ones are eliminated by means of field transformations, and the remaining couplings c_i are determined via tree-level matching. Together with the one-loop matching of the dimension five chromomagnetic interaction, this action is expected to bring the discretization errors below the one-percent level [5].

For coding, and especially for tadpole improvement of the couplings, it is convenient to write the OK action in the hopping-parameter form:

$$\begin{aligned}
 S = & \sum_x \bar{\psi}_x \psi_x - \kappa_t \sum_x \bar{\psi}_x (1 - \gamma_4) T_4 \psi_x - \kappa_t \sum_x \bar{\psi}_x (1 + \gamma_4) T_{-4} \psi_x \\
 & - \kappa_t \sum_{x,i} \bar{\psi}_x [(r_s \zeta + 8c_4) - \gamma_i (\zeta - 2c_1 - 12c_2)] T_i \psi_x
 \end{aligned}$$

$$\begin{aligned}
& - \kappa_t \sum_{x,i} \bar{\psi}_x [(r_s \zeta + 8c_4) + \gamma_i (\zeta - 2c_1 - 12c_2)] T_{-i} \psi_x \\
& + \kappa_t \sum_x \bar{\psi}_x [2c_4 + \gamma_i (c_1 + 2c_2)] T_i^2 \psi_x - \kappa_t (c_B \zeta + 16c_5) \sum_x \bar{\psi}_x i \boldsymbol{\Sigma} \cdot \mathbf{B}_{\text{lat}} \psi_x \\
& + \kappa_t \sum_x \bar{\psi}_x [2c_4 - \gamma_i (c_1 + 2c_2)] T_{-i}^2 \psi_x - \kappa_t c_E \zeta \sum_x \bar{\psi}_x i \boldsymbol{\alpha} \cdot \mathbf{E}_{\text{lat}} \psi_x \\
& + \kappa_t c_2 \sum_{x,i \neq j} \bar{\psi}_x \gamma_i \{T_i - T_{-i}, T_j - T_{-j}\} \psi_x + 2\kappa_t c_5 \sum_x \bar{\psi}_x \sum_i \sum_{i \neq j} \{i \Sigma_i B_{i\text{lat}}, (T_j + T_{-j})\} \psi_x \\
& + 2\kappa_t c_3 \sum_x \bar{\psi}_x \{\boldsymbol{\gamma} \cdot \mathbf{D}_{\text{lat}}, i \boldsymbol{\Sigma} \cdot \mathbf{B}_{\text{lat}}\} \psi_x + 2\kappa_t c_{EE} \sum_x \bar{\psi}_x \{\gamma_4 D_{4\text{lat}}, \boldsymbol{\alpha} \cdot \mathbf{E}_{\text{lat}}\} \psi_x
\end{aligned}$$

where $T_{\pm\mu} \psi(x) = U_{\pm\mu}(x) \psi(x \pm a\hat{\mu})$ with $U_{-\mu}(x) = U_{\mu}^\dagger(x - a\hat{\mu})$ and

$$m_0 a = \frac{1}{2\kappa_t} - (1 + 3r_s \zeta + 18c_4). \quad (2.1)$$

For further details and the matching conditions for the couplings c_i , we refer the reader to Ref. [5].

Given the large one-loop corrections that can arise in lattice perturbation theory [9], before using the OK action in a numerical simulation we apply tadpole improvement to the matched couplings. To carry out the tadpole improvement, it is convenient to write $T_{\pm\mu} = u_0 [T_{\pm\mu}/u_0] = u_0 \tilde{T}_{\pm\mu}$ where u_0 factors are absorbed into the couplings $\tilde{c}_i$. In this way, one finds the relations between bare and tadpole improved coefficients

$$\tilde{\kappa}_t = u_0 \kappa_t, \quad (2.2)$$

$$\tilde{r}_s \tilde{\zeta} + 8\tilde{c}_4 = r_s \zeta + 8c_4 \quad (2.3)$$

$$\tilde{\zeta} - 2\tilde{c}_1 - 12\tilde{c}_2 = \zeta - 2c_1 - 12c_2 \quad (2.4)$$

$$\tilde{c}_4 = u_0 c_4, \quad (2.5)$$

$$\tilde{c}_1 + 2\tilde{c}_2 = u_0 (c_1 + 2c_2) \quad (2.6)$$

$$\tilde{c}_2 = u_0 c_2, \quad (2.7)$$

$$\tilde{c}_B \tilde{\zeta} + 16\tilde{c}_5 = u_0^3 (c_B \zeta + 16c_5) \quad (2.8)$$

$$\tilde{c}_E = u_0^3 c_E, \quad (2.9)$$

$$\tilde{c}_3 = u_0^4 c_3, \quad (2.10)$$

$$\tilde{c}_{EE} = u_0^4 c_{EE}, \quad (2.11)$$

where the last two follow because every term in the anticommutators has five links, while one power of u_0 is absorbed, as usual, into $\tilde{\kappa}_t$. The matching conditions of Ref. [5] are then used, substituting

$$\tilde{m}_0 a = \frac{1}{2\tilde{\kappa}_t} - (1 + 3\tilde{r}_s \tilde{\zeta} + 18\tilde{c}_4) \quad (2.12)$$

for $m_0 a$. Another condition for $\tilde{c}_5$ is needed, but it is not simple to express. In the expansion of $B_{i\text{lat}}$ in terms of T s, one finds that $\bar{\psi}_x \{i \Sigma_i B_{i\text{lat}}, (T_j + T_{-j})\} \psi_x$, $j \neq i$, has terms with both 3 and 5 links. The 3-link terms arise from $T_{\pm\mu} T_{\mp\mu} = 1$. In the c_3 and c_{EE} interactions, each 3-link term appears twice, but with opposite sign, while here they have the same sign. Coding this operator with the correct u_0 factors is currently underway with USQCD software [10].

Table 1: Approximate values of the kinetic masses for the heavy-light and heavy-heavy systems obtained with the OK action. Thus, 0.042 is in the charm region and 0.036 is not yet in the bottom region.

$\tilde{\kappa}_t$	M_2^{PS} (Heavy-Light) [MeV]	M_2^{PS} (Heavy-Heavy) [MeV]
0.036	4418	7332
0.038	3500	5778
0.040	2680	4227
0.042	1876	2736

3. Simulations and Tests

We performed simulations on a “medium coarse” ($a \approx 0.15$ fm) $16^3 \times 48$ lattice with 2+1 flavors of sea quarks, $(am_l, am_s) = (0.029, 0.0484)$. From Ref. [11], we had data available with the clover action, and here we used the OK action with similar statistics, 500 configurations with 4 time sources per configuration. For the results presented here, we tadpole-improved the $\bar{\psi}_x \{i \Sigma_i B_{i\text{lat}}, (T_j + T_{-j})\} \psi_x$, $j \neq i$, interaction with $\tilde{c}_5 = u_0^4 c_5$, pending completion of the code with proper tadpole improvement. We also choose $\tilde{r}_s = \tilde{\zeta} = \tilde{c}_B = 1$. This choice fixes the value of $\tilde{c}_4$ and $\tilde{c}_5$ while the rest of the coefficients also depend on the choice of $\tilde{\kappa}_t$.

Since the action is designed to improve $O(p^4)$ terms, we need to find observables to test these improvements. One such quantity is a combination of masses introduced in Ref. [8] and later discussed in Ref. [12]. Writing the rest and kinetic meson masses $M_{1\bar{Q}q}$ and $M_{2\bar{Q}q}$ as

$$M_{1\bar{Q}q} = m_{1\bar{Q}} + m_{1q} + B_{1\bar{Q}q}, \quad (3.1)$$

$$M_{2\bar{Q}q} = m_{2\bar{Q}} + m_{2q} + B_{2\bar{Q}q}, \quad (3.2)$$

where the m s are quark masses and the B s are binding energies, Ref. [8] introduced the “inconsistency combination”

$$I := \frac{2\delta M_{\bar{Q}q} - (\delta M_{\bar{Q}Q} + \delta M_{\bar{q}q})}{2M_{2\bar{Q}q}} = \frac{2\delta B_{\bar{Q}q} - (\delta B_{\bar{Q}Q} + \delta B_{\bar{q}q})}{2M_{2\bar{Q}q}} \quad (3.3)$$

where $\delta M = M_2 - M_1$, $\delta B = B_2 - B_1$. The rightmost expression follows from the definitions.

The binding energies B_2 stem from the p^4 terms in the action [12]. By design, the the OK action improves these terms, compared with the clover action. Ideally, δB s and, hence, I should vanish, and we expect I to be smaller with an improved action. In order to compare the OK action with the clover action, we compute the rest and kinetic masses of heavy-light and heavy-heavy systems at four different hopping-parameter values, $\tilde{\kappa}_t = 0.042, 0.040, 0.038, 0.036$. Table 1 lists the obtained pseudoscalar kinetic masses, to show the range of physical mass covered here.

Figure 1 shows our results for the inconsistency I , together with results from an earlier study with the clover action [11]. For simplicity, and without serious loss in the strength of the test, we omit the light-light mass difference $\delta M_{\bar{q}q}$. As one can see, the clover action suffers from serious deviations from $I \neq 0$, especially for hopping parameters in the b -quark region. On the other hand, the OK action’s inconsistency is statistically consistent with $I = 0$ up to the largest masses considered.

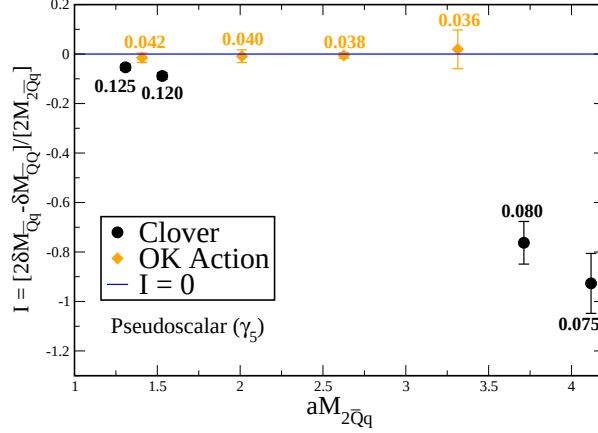


Figure 1: Comparison of the inconsistency I between the OK action and the clover action. For the clover action $\kappa = 0.122$ and $\kappa = 0.076$ correspond to tuned η_c and η_b masses.

Another way to see the effects of improvement is to look at the hyperfine splittings. Let us define

$$\Delta_1 = M_1^V - M_1^{\text{PS}}, \quad (3.4)$$

$$\Delta_2 = M_2^V - M_2^{\text{PS}}, \quad (3.5)$$

where V and PS denote vector and pseudoscalar mesons. The rest-mass splitting Δ_1 is accurate at the tree level, thanks to the clover term, but the kinetic-mass splitting Δ_2 has contributions from higher-dimension corrections such as $\{\boldsymbol{\gamma} \cdot \boldsymbol{D}, i\boldsymbol{\Sigma} \cdot \boldsymbol{B}\}$, which are improved (unimproved) with the OK (clover) action.

In Fig. 2 we plot $a\Delta_2$ vs. $a\Delta_1$ for quarkonium at the same values of $\tilde{\kappa}_t$ as above. Ideally, the data would land on the line $a\Delta_2 = a\Delta_1$. We see that the OK data fare much better than the clover data. In Fig. 3 we plot $a\Delta_2$ vs. $a\Delta_1$ for a heavy-light meson. In this case, the clover action fares well to begin with, and our statistical errors are not small enough to test whether the OK action is an improvement.

4. Outlook

Our preliminary analysis of the OK action is encouraging. It shows clear improvements in the inconsistency I and the kinetic-mass hyperfine splittings in the heavy-heavy system. For the hyperfine splitting in the heavy-light system, the improvement is not yet clear, because the clover action already works well, so a decisive test requires higher statistics. The code for the OK inverter is still under development. The next step is to finish coding of the c_5 term with the correct u_0 factors, to be followed by a thorough optimization. Thereafter, we plan on using the OK action for charm and bottom physics.

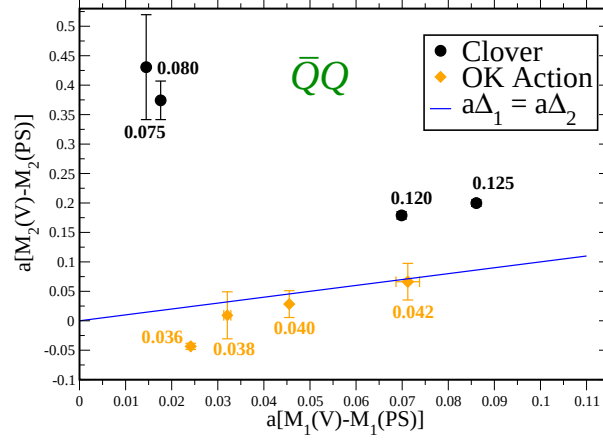


Figure 2: Kinetic-mass hyperfine splitting vs. rest-mass hyperfine splitting for the heavy-heavy system.

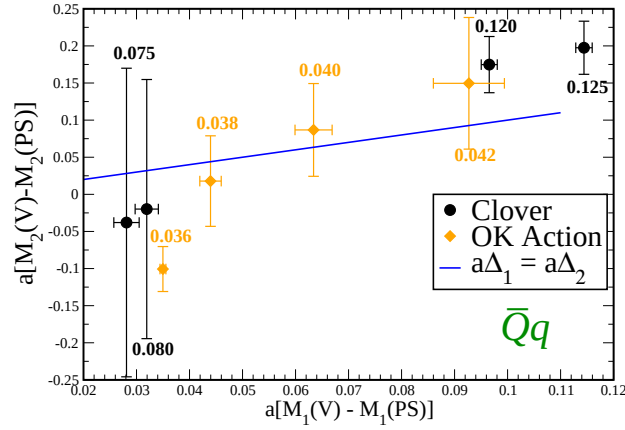


Figure 3: Kinetic-mass hyperfine splitting vs. rest-mass hyperfine splitting for the heavy-light system.

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References

- [1] A. S. Kronfeld, Nucl. Phys. Proc. Suppl. **129** (2004) 46 [arXiv:hep-lat/0310063].
- [2] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997) [arXiv:hep-lat/9604004].
- [3] B. Sheikholeslami and R. Wohlert, Nucl. Phys. B **259**, 572 (1985).
- [4] K. G. Wilson, in *New Phenomena in Subnuclear Physics*, edited by A. Zichichi (Plenum, New York, 1977).
- [5] M. B. Oktay and A. S. Kronfeld, Phys. Rev. D **78**, 014504 (2008) [arXiv:0803.0523 [hep-lat]].
- [6] A. S. Kronfeld and M. B. Oktay, PoS **LAT2006**, 159 (2006) [arXiv:hep-lat/0610069]; M. B. Oktay *et al.*, Nucl. Phys. B Proc. Suppl. **119**, 464 (2003) [arXiv:hep-lat/0209150]; **129**, 349 (2004) [arXiv:hep-lat/0310016].
- [7] A. Bazavov *et al.*, Rev. Mod. Phys. **82** (2010) 1349 [arXiv:0903.3598 [hep-lat]].
- [8] S. Collins, R. G. Edwards, U. M. Heller and J. H. Sloan, Nucl. Phys. Proc. Suppl. **47**, 455 (1996) [arXiv:hep-lat/9512026].
- [9] G. P. Lepage and P. B. Mackenzie, Phys. Rev. D **48** (1993) 2250 [arXiv:hep-lat/9209022].
- [10] <http://www.usqcd.org/>.
- [11] T. Burch *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. D **81**, 034508 (2010) [arXiv:0912.2701 [hep-lat]].
- [12] A. S. Kronfeld, Nucl. Phys. Proc. Suppl. **53**, 401 (1997) [arXiv:hep-lat/9608139].

Simulations with dynamical HISQ quarks

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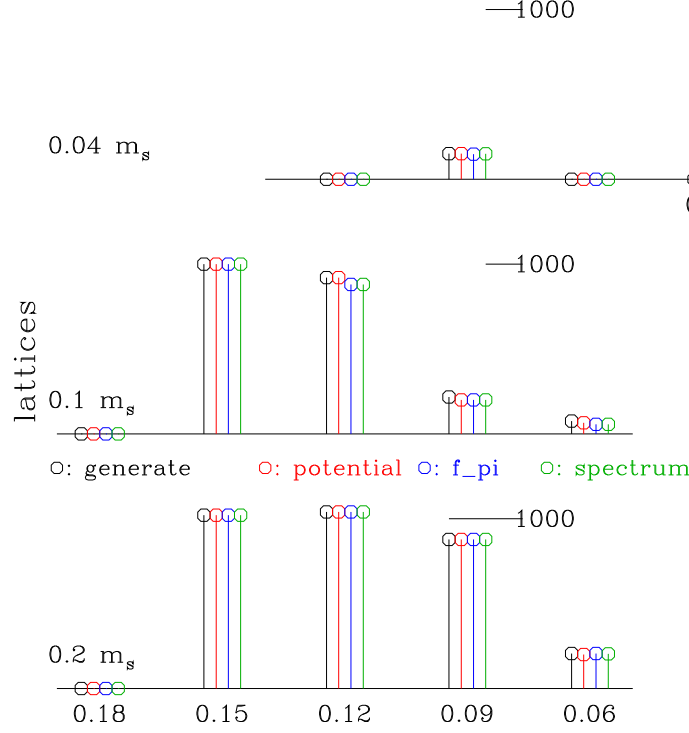
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We report on the status of a program of generating and using configurations with four flavors of dynamical quarks, using the HISQ action. We study the lattice spacing dependence of physical quantities in these simulations, using runs at several lattice spacings, but with the light quark mass held fixed at two tenths of the strange quark mass. We find that the lattice artifacts in the HISQ simulations are much smaller than those in the asqtad simulations at the same lattice spacings and quark masses. We also discuss methods for setting the scale, or assigning a lattice spacing to ensembles run at unphysical parameters.

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HISQ program, April 6, 2010

Figure 1: Status of the HISQ configuration generation program as of June 2010. We expect to eventually bring all these ensembles to approximately 1000 equilibrated configurations. The ensembles at the physical quark mass ($0.04m_s$) at $a = 0.06$ and 0.045 fm will require next generation computers. The black bars show the number of equilibrated configurations, and the red, blue and green bars show the progress of static potential, light pseudoscalar amplitudes, and simple hadron spectrum calculations. These are being done in parallel with the configuration generation to the extent possible.

1. Introduction

During the past eleven years the MILC collaboration has carried out a program of QCD simulations using an improved staggered quark action, the “asqtad” action. This action has lattice artifacts that are much smaller than those in the original (one-link) staggered quark action. These simulations used two light and one strange dynamical quarks. Lattices have been generated with spacings ranging from 0.18 fm to 0.045 fm and light quark masses ranging from $0.05 m_s$ to m_s . The spatial sizes of these lattices ranged from 2.5 fm to 5.8 fm. In total, around 25000 configurations have been archived. These configurations have been used for a wide variety of QCD studies and are all publicly available from the NERSC Gauge Connection archive, from ILDG, or informally. A detailed review of this simulation program can be found in Ref. [1].

Recently the HPQCD/UKQCD collaboration introduced a “highly improved staggered quark” (HISQ) action which further reduces taste symmetry violations, which are expected to be the largest lattice artifacts with staggered quark actions. Using this action, and taking advantage of improved machine power and algorithm development, we have begun a new program of lattice QCD simu-

lations. There are several differences between this new set of simulations and those in the asqtad program. First, the smeared links used in the $\mathcal{D}$ operator are done with a two level smearing, so that the quarks effectively see a smoother lattice, leading to reduced taste symmetry violations. Second, the three-link (Naik) term in $\mathcal{D}$ for the charm quark is modified to improve the dispersion relation of the free charm quark. These two improvements together make up what is usually called the HISQ action[2]. In addition, this generation of simulations is using spatial lattice sizes about 20% larger than the comparable asqtad action simulations. While this seems like a small adjustment, since finite size effects are expected to decrease as $\exp(-m_\pi L)$, these effects should be significantly reduced. Also, the Symanzik improved gauge action contains the one-loop effects of the HISQ fermions[3]. The comparable asqtad effects were not available when that program was started, but turned out to be surprisingly large[4]. With experience from the asqtad simulations, we expect to do a better job of tuning the dynamical quark masses, reaching a level of perhaps 2% accuracy. In contrast, some of the early asqtad lattice ensembles had strange quark masses as much as 20% off their *a posteriori* correct value. Finally, we are including a dynamical charm quark. At our smaller lattice spacings, am_c is not large. We do expect the effects of dynamical charm to be small in most cases, but they may be important to the high temperature QCD part of our program, and they are quite cheap to include.

In this program we expect to produce full scale ensembles with about 1000 equilibrated configurations at lattice spacings of 0.15, 0.12, 0.09 and 0.06 fm, with light quark masses of $m_s/5$, $m_s/10$ and the physical value, roughly $m_s/27$. In the not too distant future we also expect to generate an ensemble with $a = 0.045$ fm and the physical quark masses. We will also generate a number of coarser ensembles, mainly for setting the scale in HISQ high temperature QCD simulations. For each of these approximate lattice spacings we are using values of $10/g^2$ and u_0 determined from the $m_l = m_s/5$ runs at all light quark masses. The strange and charm quark masses are adjusted from short tuning runs to give the physical values of $2M_K^2 - M_\pi^2$ and $\frac{3}{4}M_\Psi + \frac{1}{4}M_{\eta_c}$ respectively. Figure 1 shows the current (June 2010) status of these runs.

2. Tests of scaling

The first stage in this program was to generate complete ensembles at a fixed but unphysical light quark mass of $m_s/5$ at lattice spacings of 0.15, 0.12 and 0.09 fm. This allows us to test scaling, or dependence of calculated quantities on the lattice spacing. In particular, we wish to see if the reductions in taste symmetry violations are accompanied by reductions in lattice spacing dependence of other quantities. The results of these tests are briefly summarized here, but a complete report may be found in Ref. [5].

The HPQCD/UKQCD collaboration demonstrated the reduction of taste violations with HISQ valence quarks using quenched and asqtad sea quarks[2]. As expected, we find similar results with HISQ sea quarks. Figure 2 shows results for the taste splittings with HISQ valence and sea quarks with $m_l = m_s/5$, including some results on a partially completed ensemble with $a = 0.06$ fm.

Perhaps the most stringent test of improvement is the topological susceptibility, since the dependence of this quantity on the sea quark mass demonstrates that the sea quarks are modifying the gluon configurations. Figure 3 shows the topological susceptibility for most of the asqtad ensembles[7], together with the HISQ results for $m_l = m_s/5$ at $a = 0.12$ and 0.09 fm. It can be seen

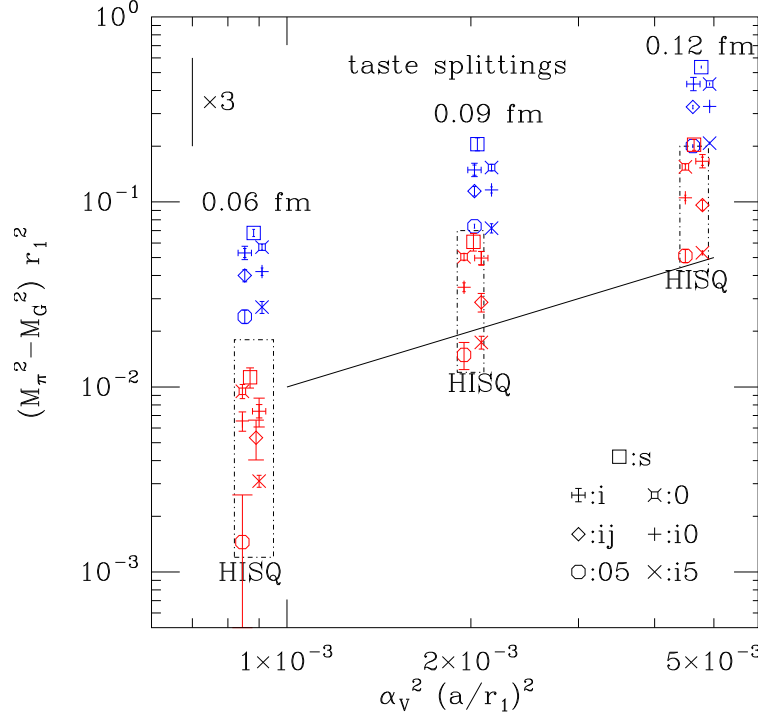


Figure 2: Taste splittings among the pions, comparing the asqtad and HISQ actions. The asqtad results used configurations with 2+1 flavors of dynamical quarks, and the HISQ results 2+1+1 flavors. The quantity plotted is $r_1^2 (M_\pi^2 - M_G^2)$, where M_π is the mass of the non-Goldstone pion and M_G is the mass of the Goldstone pion. Reading from top to bottom, the non-Goldstone pions are the π_s (box), π_0 (fancy box), π_i (fancy plus), π_{i0} (plus), π_{ij} (diamond), π_{i5} (cross) and π_{05} (octagon). $r_1^2 (M_\pi^2 - M_G^2)$ is known to be almost independent of the light-quark mass. The vertical bar at the upper left shows the size of a factor of three, roughly the observed reduction in taste splittings, while the sloping solid line shows the theoretically expected dependence on lattice spacing. Nearly degenerate points have been shifted horizontally to improve their visibility.

that the HISQ points fall below the corresponding asqtad points, which are indicated by the arrows in the figure. Note that the HISQ points are to the left of the corresponding asqtad points. This is because the horizontal axis is the mass of the taste singlet pion (the heaviest pion taste), and the reduction in taste symmetry breaking moves the points to the left. It is the movement down relative to the asqtad points that represents an improvement in the gluon configurations.

We also looked at the masses of the ρ and nucleon in these ensembles. Strictly, these are an unphysical vector meson and baryon with both valence and sea light quark masses at $m_s/5$. Thus, we can check their dependence on lattice spacing, but without a chiral extrapolation we cannot test their masses against experiment. With this caution, we found that the dependence of $r_1 M_\rho$ and $r_1 M_N$ on the lattice spacing was much smaller than for the asqtad ensembles at comparable quark masses. More details are in Ref. [5]. Of course, this could be interpreted either as improved scaling of hadron masses using r_1 to set the scale or improved scaling of r_1 using hadron masses to set the scale.

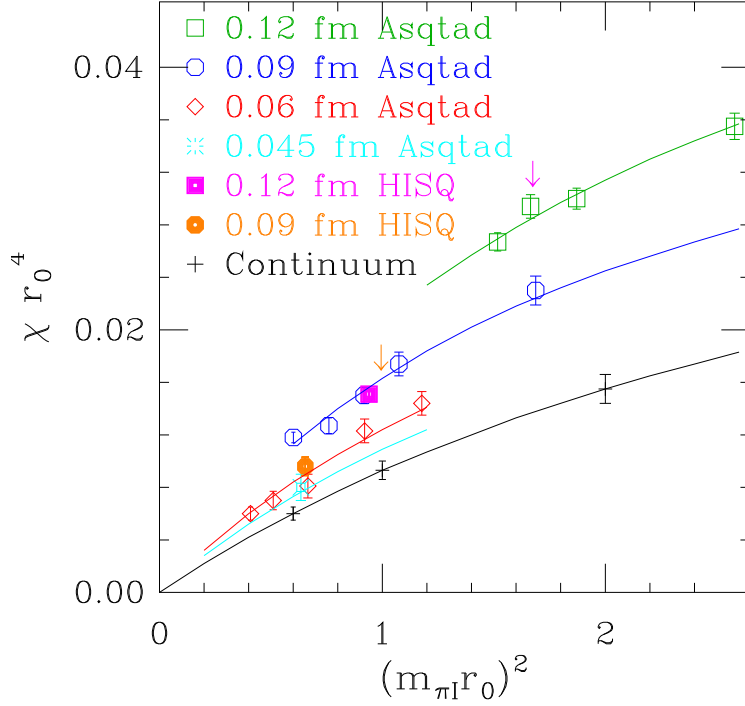


Figure 3: The topological susceptibility, comparing the asqtad and HISQ actions. Points with the asqtad action are shown for several lattice spacings and quark masses, and the HISQ results for $a \approx 0.12$ fm and $a \approx 0.09$ fm with $m_l = 0.2m_s$. For the horizontal axis we use the mass of the taste singlet pion, since in lowest order chiral perturbation theory the topological susceptibility is a function of this mass [6]. The curves in the figure come from a chiral perturbation theory fit to the asqtad data. A discussion of the methods used for computing the susceptibility and the asqtad results can be found in Ref. [7]. The two arrows indicate the locations of asqtad points with lattice spacing and quark mass similar to the two HISQ points. (In the case of the $a \approx 0.09$ fm HISQ point, the quark mass falls between two of the masses of the asqtad points.)

3. Setting the length scale

QCD simulation programs involving unphysical quark masses generally involve a definition of the lattice spacing as a function of the gauge couplings and sea quark masses. About the only real requirement on this definition is that it should be correct at the physical quark masses in the continuum limit. The most common choice is a scale determined from the static quark potential[8], usually either $r_0^2 F(r_0) = -1.65$ or $r_1^2 F(r_1) = -1$. This is not a physical quantity, but it is a convenient interpolating quantity that can be determined accurately with a reasonable amount of work. Its value is determined by matching some physical quantity, such as quarkonium mass splittings or f_π , in the continuum and chiral limits. Recently the HPQCD collaboration has suggested using the decay constant of a fictitious isovector pseudoscalar meson with valence quark masses equal to the strange quark mass as the length standard[9], which we will call f_{ss} . Like r_0 or r_1 , this is an unphysical quantity whose value is determined by matching a physical quantity, most likely f_π , in the continuum limit at the physical quark mass. Of course, one could use any mass for the valence

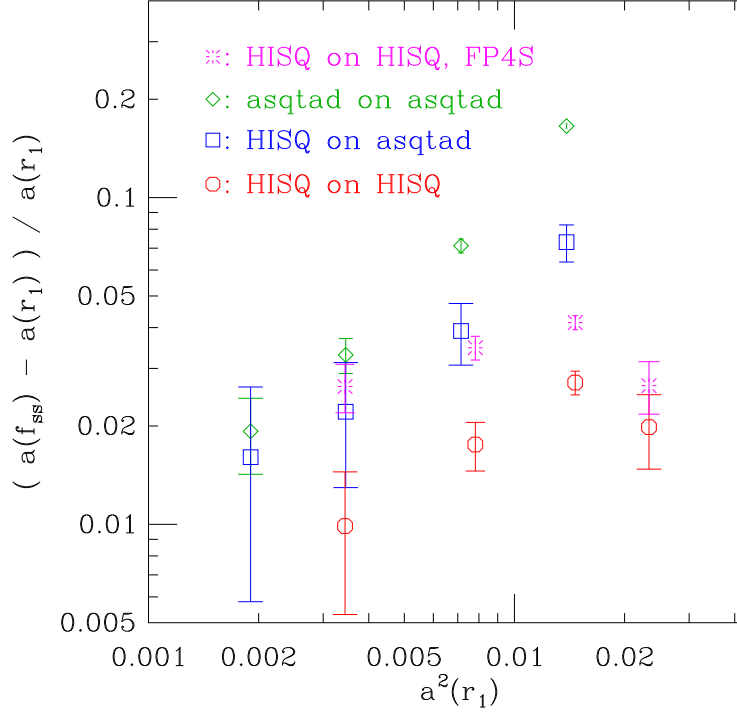


Figure 4: Differences in determinations of the length scale using different standards. In the legend, the symbol types are labelled as “valence on sea”. The “FP4S” points (bursts) use a pseudoscalar meson with both valence quarks at 0.4 times the strange quark mass, while all the other points use valence quarks at the strange quark mass. The “HISQ on asqtad” points are taken from Ref. [9].

quark, and we have been experimenting with using a mass of 0.4 times the strange quark mass. The choice of reference mass involves a tradeoff — we want a mass heavy enough so that an accurate simulation result is possible but light enough so that chiral perturbation theory can be used with confidence.

Use of an unphysical decay constant has several advantages. It is possible to get very good accuracy, and the systematic errors from things like choices of fit ranges are better understood than those in r_1 . Also, for calculations involving hadron masses and matrix elements, there are fewer steps in the logic relating the lattice results to dimensionful quantities. On the other hand, the meson decay constant takes much more computer time than the static quark potential (although it may be needed anyway) and is dependent on the choice of valence quark formulations. For example, asqtad and HISQ valence quarks would give different lattice spacings for the same ensemble of configurations.

Table 1 shows the lattice spacings for several asqtad and HISQ ensembles determined from r_1 and from pseudoscalar amplitudes with asqtad and HISQ valence quarks. Figure 4 shows the differences between the pseudoscalar and r_1 lattice spacings versus a^2 , including lattice spacings determined from both f_{ss} and f_{4s} , and it can be seen that the differences are vanishing in the continuum limit.

Action	$10/g^2$	am_l	am_s	am_c	$a(r_1)$	$a(f_{ss,asq})$	$a(f_{ss,HISQ})$
asqtad	6.76	0.01	0.05	–	0.1178(2)	0.1373(2)	0.1264 (11)
asqtad	7.09	0.0062	0.031	–	0.0845(1)	0.0905(3)	0.0878(7)
asqtad	7.46	0.0036	0.018	–	0.0588(2)	0.0607(1)	0.0601(5)
asqtad	7.81	0.0028	0.014	–	0.0436(2)	0.0444(1)	0.0443(4)
HISQ	5.80	0.013	0.065	0.838	0.1527(7)	na	0.1558(3)
HISQ	6.00	0.0102	0.0509	0.635	0.1211(2)	na	0.1244(2)
HISQ	6.30	0.0074	0.037	0.440	0.0884(2)	na	0.0900(1)

Table 1: Lattice spacing determinations by various methods. The values for HISQ valence quarks with asqtad sea quarks are taken from Ref. [9]. In the other cases, the errors are statistical only; they do not include the errors on the physical value of r_1 ($r_1 = 0.3108(15)(^{+26}_{-79})$) or on the estimate of f_{ss} in MeV, $f_{ss} = 181.5(1.0)$ MeV[9].

Acknowledgments

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References

- [1] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010), [arXiv:0903.3598].
- [2] E. Follana *et al.*, Nucl. Phys. B (Proc. Suppl.) **129** and **130**, 447 (2004), [arXiv:hep-lat/0311004];
E. Follana *et al.*, Nucl. Phys. B (Proc. Suppl.) **129** and **130**, 384, 2004. [arXiv:hep-lat/0406021];
E. Follana *et al.* [HPQCD Collaboration and UKQCD Collaboration], Phys. Rev. D **75**, 054502 (2007) [arXiv:hep-lat/0610092].
- [3] A. Hart, G. von Hippel and R.R. Horgan, Phys. Rev. D **79**, 074008 (2009), [arXiv:0812.0503].
- [4] Zh. Hao *et al.* Phys. Rev. **D76**, 034507 (2007), [arXiv:0705.4660].
- [5] A. Bazavov *et al.*, Phys. Rev. D **82**, 074501 (2010), [arXiv:1004.0342].
- [6] C. Aubin and C. Bernard, Phys. Rev. **D68**, 034014, (2003), [arXiv hep-lat/0304014]; B. Billeter, C.E. DeTar and J. Osborn, Phys. Rev. **D70**, 077502, (2004), [arXiv hep-lat/0406032].
- [7] A. Bazavov *et al.*, Phys. Rev. **D81**, 114501 (2010), [arXiv:1003.5695].
- [8] R. Sommer, Nucl. Phys. **B411**, 839 (1994), [arXiv:hep-lat/9310022].
- [9] C.T.H. Davies *et al.*, Phys. Rev. D **81**, 034506 (2010), [arXiv:0910.1229].

CHARMONIUM SPECTROSCOPY FROM LATTICE QCD*

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I give a short review of the current status of lattice QCD calculations of the spectrum of charmonium.

I. INTRODUCTION

In recent years the numerical simulation of lattice quantum chromodynamics (QCD) has developed into an enormously successful method for obtaining precise values of several Standard Model parameters. It is the only truly *ab initio* method available for doing nonperturbative studies of QCD. It provides a unified framework for treating mesons and baryons involving charm and bottom quarks, whether in a heavy-light or heavy-heavy configuration.

For charm physics the primary phenomenological objectives of lattice QCD are to help in the discovery and characterization of excited states, including exotics, to determine decay constants[1, 2] and form factors, and to calculate electromagnetic transition rates. Theoretical objectives include providing guidance for effective field theory.

Since the last Charm conference there have been no new comprehensive numerical lattice studies of exotics and excited quarkonium states. So I will review the current status only briefly. There has been exciting progress, however, in the high precision determination of masses of several of the lowest lying states involving heavy quarks. Progress here is, of course, prerequisite to an accurate determination and characterization of excited states.

Lattice simulations have their limitations. While static properties, including masses and matrix elements are relatively easy to calculate, scattering processes, including charmonium production, inclusive processes, and multihadronic (more than two-body) decays are very difficult.

In addition to the usual challenges of extrapolating to the continuum and physical light quark masses, heavy quark simulations face special difficulties. The lattice spacing a introduces a momentum cut off of order $1/a$, typically less than $2 - 3$ GeV with today's lattices. As the quark mass M approaches the cut off, discretization errors grow. Such mass-related errors can be controlled by a suitable formulation of the Dirac action for the heavy quark. Among them are (1) a lattice

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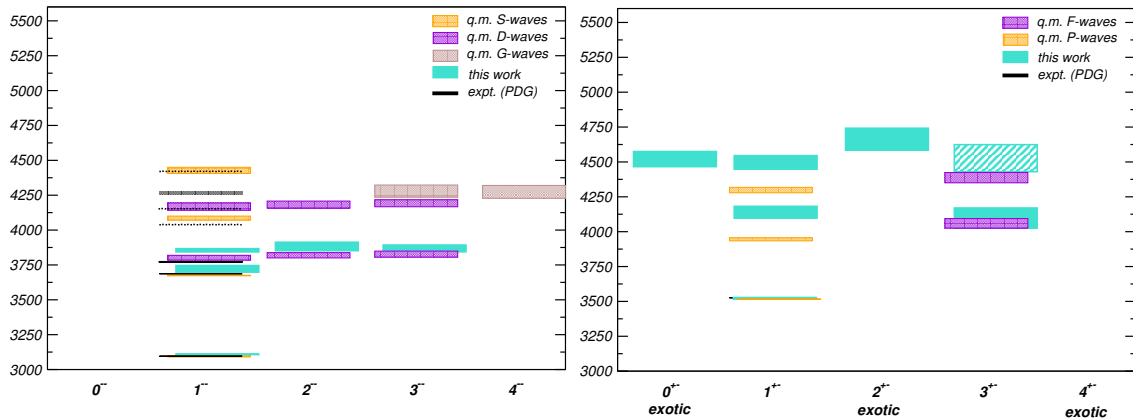


FIG. 1: Charmonium excitation spectrum in MeV from Ref. [7]. Left: J^{--} states. Right J^{+-} states including exotics. Lattice results (blue) are compared with PDG values (black) and various quark model results (purple and orange). Color online.

version of nonrelativistic QCD[3], which converges rather slowly for charm, but well for bottom, (2) the Fermilab action[4] and its improvements[5, 6], good for both charm and bottom, and (3) the highly improved staggered quark action (HISQ) with discretization errors of order $\mathcal{O}(\alpha_s^2(aM_c)^2)$, good for charm, but not so good for bottom with today’s lattices.

II. EXCITATION SPECTRUM AND EXOTICS

In 2008 Dudek *et al.*[7] published results of a comprehensive lattice QCD study of the excitation spectrum of charmonium. In order to access excited states they introduced a large set of interpolating operators and used a “variational” method to determine their masses.

How well does this work? Figure 1 (left) gives an impression. Consider the 1^{--} channel, where the ground state J/ψ has a very clean signal. Six states were found, but only the first three shown were unambiguous enough that the authors were willing to associate them with known levels, namely the J/ψ , $\psi(2S)$ and $\psi(3S)$. The lattice levels were generally higher than experiment and the discrepancies grew from 12 to 82 MeV. They were also higher than quark model determinations, as shown. In the $PC = +-$ channel this study also produced a couple spin-exotic states as shown in Fig. 1. See Ref. [7] for more states.

These results are pioneering, but they are deficient for a number of reasons. Sea quark effects were omitted, the calculation was done at only one lattice spacing, so an extrapolation to the continuum is not possible, and open charm states were ignored. The Hadron Spectrum Collaboration is remedying these shortcomings[8].

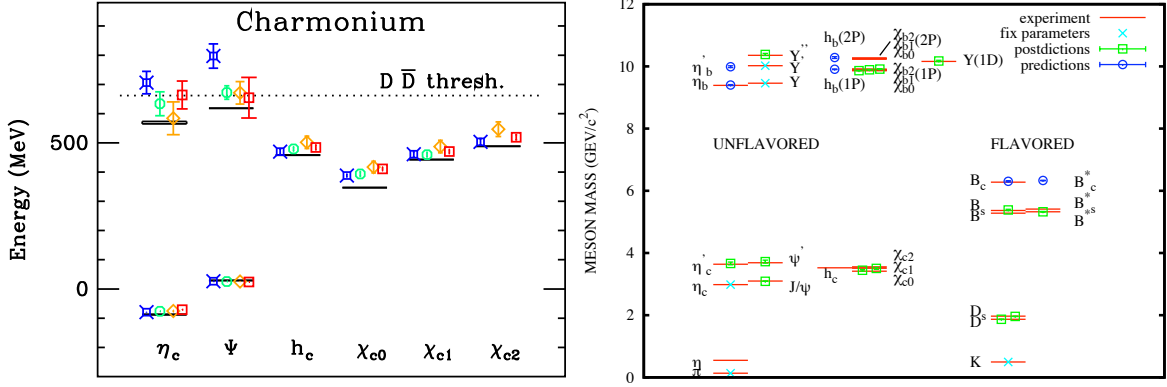


FIG. 2: Left: Charmonium levels from Ref. [10] based on splittings from the spin-averaged $1S$ level with quark masses determined from the D_s and light pseudoscalar mesons and scale determined from upslon splittings. Results for four lattice spacings from 0.18 fm (red) to 0.09 fm (blue) are shown. Black lines are PDG values. Right: complete low-lying heavy and light meson spectrum from Ref. [11] showing five masses used to fix four quark masses and the lattice scale and three masses predicted in advance of experiment.

To include sea quarks and allow extrapolation to the continuum and to physical light quark masses requires generating gauge field configurations (ensembles) with various lattice spacings and light quark mass combinations. The MILC collaboration makes publicly available a large archive of such ensembles with lattice spacing ranging from 0.15 fm to 0.045 fm and light quark mass ratios m_{ud}/m_s ranging down to 0.05, compared with the physical value of approximately 0.037[9].

MILC gauge configurations are being used by the FNAL/MILC and HPQCD collaborations to study the quarkonium spectrum. The FNAL/MILC campaign currently uses Fermilab quarks for both charm and bottom and HPQCD uses HISQ charm quarks and NRQCD bottom quarks. Most of the FNAL/MILC results presented here are from last year's study[10], which, like the HPQCD study, used a limited set of interpolating operators and looked at only the low-lying states. A new FNAL/MILC campaign currently under way is aimed at excited as well as ground states using a large set of interpolating operators, higher statistics, smaller lattice spacings, and more accurate heavy quark mass tuning. I will give a preview of the improvement we hope to obtain.

III. LOW-LYING LEVELS

Broadly speaking, lattice simulations do quite well reproducing the low-lying hadronic states. Figure 2 gives an overview of the charmonium spectrum of the FNAL/MILC collaboration (left) [10] and the full gold-plated meson spectrum of the HPQCD collaboration[11] (right). To appreciate the precision of the calculation, we turn to a finer mass scale in the remainder of this minireview.

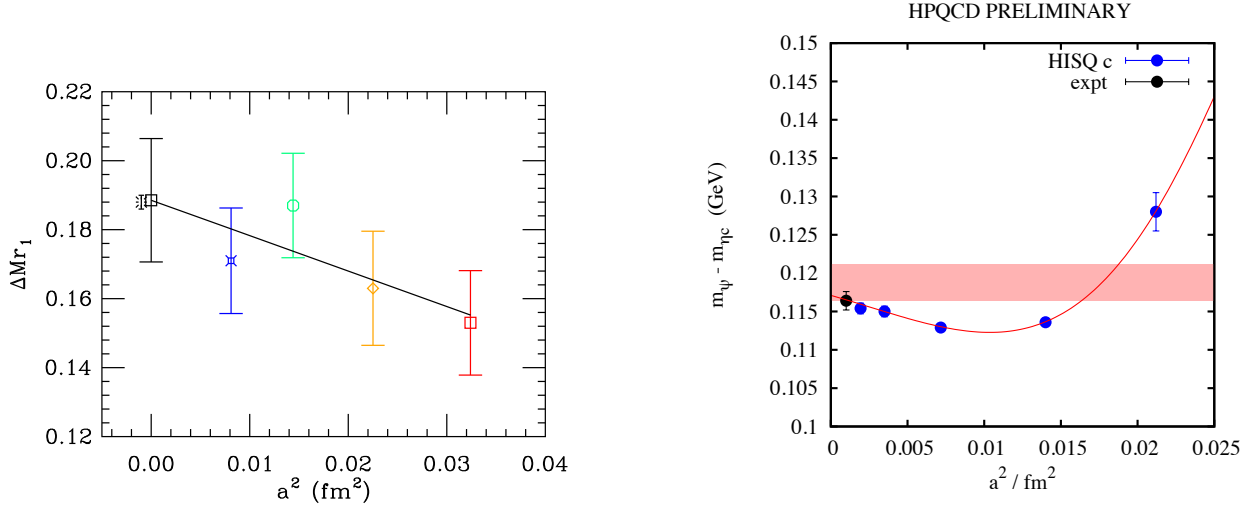


FIG. 3: Hyperfine splitting in charmonium extrapolated to zero lattice spacing. PDG values are in black. Left: FNAL/MILC[10]. Units are $r_1 \approx 1.58 \text{ GeV}^{-1}$. Right: HPQCD[12].

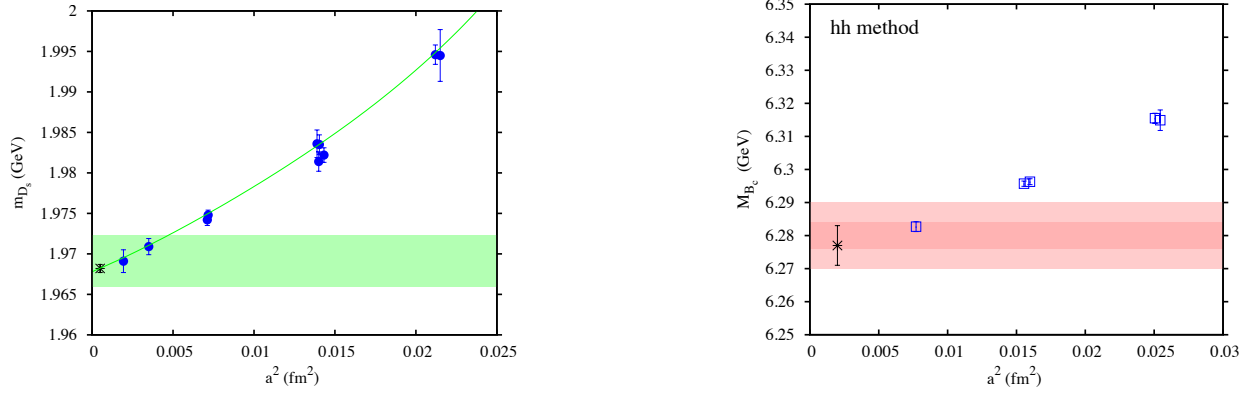


FIG. 4: Recent HPQCD results for the D_s mass (left)[14] and B_c (right)[15].

Historically, the hyperfine splitting of the $1S$ state has proven to be a stringent test of lattice methodology. In Fig. 3 recent results of the FNAL/MILC collaboration (left) [10] are compared with still more recent results of the HPQCD collaboration (right)[12]. The FNAL/MILC calculation was based on Fermilab quarks. The extrapolated value is 117(11) MeV. In this result annihilation effects are not included. The HPQCD result is based on HISQ charm quarks. The pink band indicates the full error budget (± 2 MeV), and includes a small increase due to annihilation, as suggested by perturbation theory. Determining level shifts due to annihilation is difficult. A recent nonperturbative (lattice) result estimates, instead, a decrease of $1 - 4$ MeV from charm annihilation[13]. Thus, apparently, we have reached the point where annihilation effects cannot be ignored.

Further examples of achievable precision in gold-plated quantities are shown in Fig. 4. The D_s

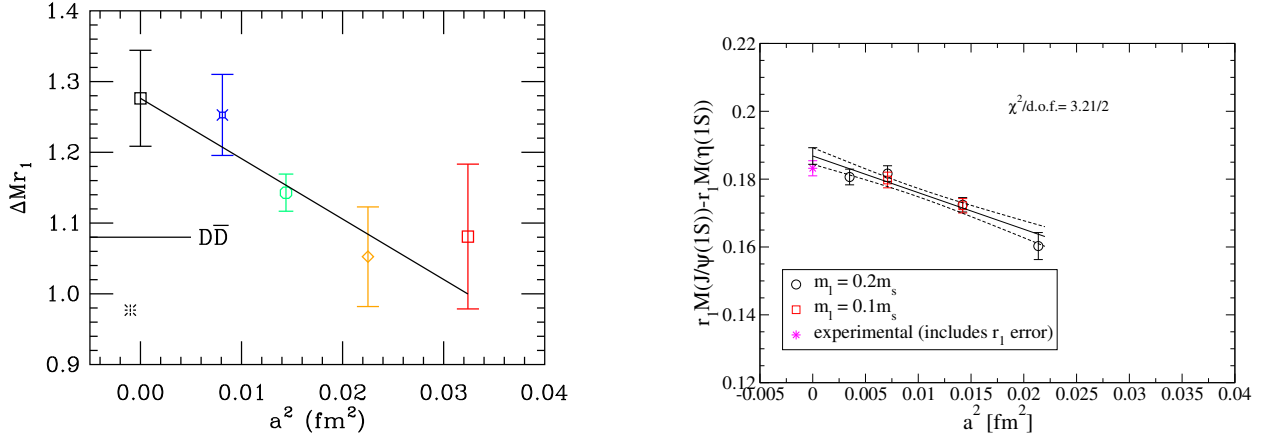


FIG. 5: Left: $\overline{2S} - \overline{1S}$ splitting from Ref. [10] showing possible complications from open charm. Right: Sample FNAL/MILC preliminary result for the $1S$ hyperfine splitting from the new analysis with much reduced errors.

mass is obtained to 3 MeV accuracy from the mass splitting $M(c\bar{s}) - \frac{1}{2}M(\eta_c)$ [14], and the B_c mass is obtained to 10 MeV accuracy from the splitting $M(B_c) - M(b\bar{b})/2 - M(\eta_c)/2$ [15].

Going beyond gold-plated quantities, the FNAL/MILC simulation results for the spin-averaged $2S - 1S$ splitting, shown in Fig. 5 (left) disagrees with the experimental value[10]. Could this be a result of complications from the nearby open charm threshold? Those simulations do not currently treat two-body scattering states. A recent calculation by Bali and Ehmman with a small basis set suggests that they may be important for even states well below threshold, but further study is needed[16].

IV. CONCLUSIONS AND OUTLOOK

We have seen dramatic improvement in our ability to reproduce the masses of the lowest lying charmonium states. This has been brought about by the use of improved quark actions, higher statistics, accurate tuning of the heavy quark masses, smaller lattice spacing, and the availability of gauge field ensembles that support an extrapolation to physical sea quark masses and zero lattice spacing. New analysis campaigns with multiple interpolating operators are underway both by the Hadron Spectrum Collaboration and the Fermilab Lattice/MILC collaborations. A preview of the hyperfine splitting from this new analysis is shown in Fig. 5 (right), a considerable improvement over Fig. 3 (left). These campaigns should provide more accurate information about excited and

exotic states. Treating two-body scattering states will continue to be a long-term challenge.

- [1] J. Simone, these proceedings.
- [2] Hee Chang Na, these proceedings.
- [3] G. P. Lepage *et al.*, Phys. Rev. D **46**, 4052 (1992) [arXiv:hep-lat/9205007].
- [4] A. X. El-Khadra, A. S. Kronfeld and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997) [arXiv:hep-lat/9604004].
- [5] M. B. Oktay and A. S. Kronfeld, Phys. Rev. D **78**, 014504 (2008) [arXiv:0803.0523 [hep-lat]].
- [6] M. B. Oktay, PoS LAT2010 (to be published).
- [7] J. J. Dudek *et al.*, Phys. Rev. D **77**, 034501 (2008) [arXiv:0707.4162 [hep-lat]].
- [8] S. Ryan, PoS LAT2010 (to be published).
- [9] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010) [arXiv:0903.3598 [hep-lat]].
- [10] T. Burch *et al.*, Phys. Rev. D **81**, 034508 (2010) [arXiv:0912.2701 [hep-lat]].
- [11] E. B. Gregory *et al.*, Phys. Rev. Lett. **104**, 022001 (2010) [arXiv:0909.4462 [hep-lat]].
- [12] E. Follana (HPQCD Collaboration) PoS LAT2010 (to be published).
- [13] L. Levkova and C. DeTar, arXiv:1012.1837 [hep-lat].
- [14] C. T. H. Davies *et al.*, arXiv:1008.4018 [hep-lat].
- [15] E. B. Gregory *et al.*, arXiv:1010.3848 [hep-lat].
- [16] G. Bali and C. Ehmman, arXiv:0911.1238 [hep-lat].

Semileptonic B to D decays at nonzero recoil with 2+1 flavors of improved staggered quarks

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The Fermilab Lattice-MILC collaboration is completing a comprehensive program of heavy-light physics on the MILC (2+1)-flavor asqtad ensembles with lattice spacings as small as 0.045 fm and light-to-strange-quark mass ratios as low as 1/20. We use the Fermilab interpretation of the clover action for heavy valence quarks and the asqtad action for light valence quarks. The central goal of the program is to provide ever more exacting tests of the unitarity of the CKM matrix. We give a progress report on one part of the program, namely the analysis of the semileptonic decay B to D at both zero and nonzero recoil. Although final results are not presented, we discuss improvements in the analysis methods, the statistical errors, and the parameter coverage that we expect will lead to a significant reduction in the final error for $|V_{cb}|$ from this decay channel.

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*Speaker.

1. Introduction

Precision tests of the standard model from flavor factory and intensity frontier experiments can reveal new physics even if the accelerator energy isn't sufficient to create the new particles associated with the new physics. Here preliminary results of a lattice-QCD calculation of the nonzero-recoil form factor for the semileptonic process $B \rightarrow D\ell\bar{\nu}$ are presented. The principal goal is to determine $|V_{cb}|$ to a high precision. The theoretical uncertainty on $|V_{cb}|$ limits the precision of the unitarity triangle constraint from neutral kaon mixing.

There are several methods for determining $|V_{cb}|$. (1) From the inclusive decay $b \rightarrow c\ell\bar{\nu}$, perturbation theory and the operator product expansion provide an estimate of the inclusive decay rate, which is then combined with the measured decay rate to obtain $|V_{cb}|$ [1]. (2) From the exclusive semileptonic decay $B \rightarrow D^*\ell\bar{\nu}$, lattice-QCD methods provide the hadronic contribution to the decay rate [2]. For the special case of zero recoil, we have presented an unquenched calculation for this process three years ago [3] with a preliminary update reported at the Lattice 2010 [4] and CKM 2010 conferences [5] (3) Likewise, from the exclusive semileptonic decay $B \rightarrow D\ell\bar{\nu}$, lattice-QCD methods provide the hadronic contribution [8]. Here we report the first unquenched lattice-QCD calculation for this process at nonzero recoil.

At present there is a 1.6σ disagreement between the value of $|V_{cb}|$ determined from inclusive decays and our recent preliminary value based on the decay $B \rightarrow D^*\ell\bar{\nu}$ at zero recoil, as illustrated in Fig. 1. Thus, further cross checks of and improvements in the theoretical calculations are needed. The value of $|V_{cb}|$ can be determined from the ratio of the measured decay rate to the calculated hadronic form factor at any chosen recoil energy. Typically, the uncertainty in the experimental measurement increases as the recoil energy vanishes [12], whereas the uncertainty in the lattice-QCD calculation decreases [6, 7, 8]. Thus, to minimize the uncertainty in the ratio, it is best to combine results of the experimental measurement with those of the lattice-QCD calculation over the full range of available recoil energies. For this reason we undertake an analysis over a broad range.

2. Methodology for determining $|V_{cb}|$

The hadronic weak matrix element for this process is commonly parameterized as

$$\langle D(p') | \gamma_\mu | B(p) \rangle = \sqrt{m_B m_D} [h_+^{B \rightarrow D}(w)(v + v')_\mu + h_-^{B \rightarrow D}(w)(v - v')_\mu] . \quad (2.1)$$

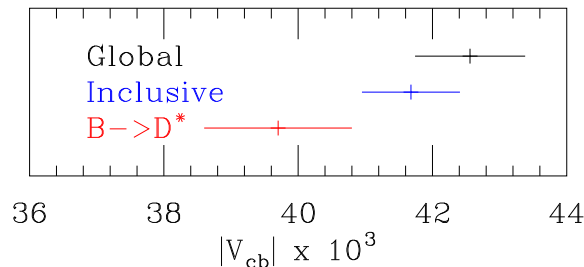


Figure 1: The central values and errors resulting from three determinations of $|V_{cb}|$: (1) A “global fit” to the unitarity triangle including all inputs except $|V_{cb}|$ [9] [10], (2) inclusive measurements summarized by the HFAG [11], and (3) our $B \rightarrow D^*$ lattice-QCD calculation [4, 5].

Here, w is velocity transfer, $w = v \cdot v'$. The differential rate for the semileptonic decay $B \rightarrow D \ell \bar{\nu}$ is

$$\frac{d\Gamma(B \rightarrow D l \bar{\nu})}{dw} = \frac{G_F^2 |V_{cb}|^2}{48\pi^3} (m_B + m_D)^2 m_D^3 [w^2 - 1]^{3/2} |\mathcal{G}_{B \rightarrow D}(w)|^2, \quad (2.2)$$

where $\mathcal{G}_{B \rightarrow D}(w)$ is defined as

$$\mathcal{G}_{B \rightarrow D}(w) = h_+^{B \rightarrow D}(w) - \frac{m_B - m_D}{m_B + m_D} h_-^{B \rightarrow D}(w). \quad (2.3)$$

Thus, once we know $h_+^{B \rightarrow D}$ and $h_-^{B \rightarrow D}$, we can determine the form factor $\mathcal{G}_{B \rightarrow D}(w)$. Then, combining it with the result of the decay rate from experiment, we will obtain $|V_{cb}|$. In order to construct $h_+^{B \rightarrow D}$ and $h_-^{B \rightarrow D}$, we need the following quantities:

$$h_+(w) = R_+(\mathbf{p})[1 - x_f(\mathbf{p})R_-(\mathbf{p})], \quad (2.4)$$

$$h_-(w) = R_+(\mathbf{p})[1 - R_-(\mathbf{p})/x_f(\mathbf{p})], \quad (2.5)$$

$$R_+(\mathbf{p}) = \langle D(\mathbf{p}) | \mathcal{V}^4 | B(0) \rangle, \quad (2.6)$$

$$R_-(\mathbf{p}) = \frac{\langle D(\mathbf{p}) | \mathcal{V}^1 | B(0) \rangle}{\langle D(\mathbf{p}) | \mathcal{V}^4 | B(0) \rangle}, \quad (2.7)$$

$$x_f(\mathbf{p}) = \frac{\langle D(\mathbf{p}) | \mathcal{V}^1 | D(0) \rangle}{\langle D(\mathbf{p}) | \mathcal{V}^4 | D(0) \rangle}, \quad (2.8)$$

where $\mathcal{V}^\mu$ is the continuum hadronic weak vector current.

In our calculation we use the local (nonconserved) lattice vector current $V_\mu(x) = \bar{\Psi}_b(x) i\gamma_\mu \Psi_c(x)$ with $\mathcal{O}(a)$ improved heavy quark fields $\Psi_h(x)$ following [13], and we renormalize it following a partly nonperturbative method, namely

$$Z_{Vbc} = \rho_V \sqrt{Z_{Vbb} Z_{Vcc}}, \quad (2.9)$$

where the flavor-diagonal renormalization coefficients are computed nonperturbatively on the lattice via the conditions

$$Z_{Vbb} \langle B | V^4 | B \rangle = 1, \quad (2.10)$$

$$Z_{Vcc} \langle D | V^4 | D \rangle = 1, \quad (2.11)$$

and ρ_V is computed perturbatively [7]. Because of cancellations among similar loop diagrams, we expect that ρ_V is nearly equal to 1 [7]. Preliminary results presented here omit the ρ_V factor.

At zero recoil ($w = 1$) we use the double ratio method [2]:

$$|h_+(1)|^2 = \rho_V^2 \frac{\langle D | V^4 | B \rangle \langle B | V^4 | D \rangle}{\langle D | V^4 | D \rangle \langle B | V^4 | B \rangle}. \quad (2.12)$$

This ratio suppresses a large part of the statistical fluctuations, and it builds in the current renormalization $\sqrt{Z_{Vbb} Z_{Vcc}}$.

$a(\text{fm})$	size	m_l/m_h	$a(\text{fm})$	size	m_l/m_h
≈ 0.15	$16^3 \times 48$	0.2	$\approx \mathbf{0.09}$	$40^3 \times 96$	0.1
$\approx \mathbf{0.12}$	$20^3 \times 64$	0.14	≈ 0.09	$64^3 \times 96$	0.05
$\approx \mathbf{0.12}$	$20^3 \times 64$	0.2	≈ 0.06	$48^3 \times 144$	0.2
$\approx \mathbf{0.12}$	$20^3 \times 64$	0.4	≈ 0.06	$48^3 \times 144$	0.4
$\approx \mathbf{0.12}$	$24^3 \times 64$	0.1	≈ 0.06	$56^3 \times 144$	0.14
$\approx \mathbf{0.09}$	$28^3 \times 96$	0.2	≈ 0.06	$64^3 \times 144$	0.1
$\approx \mathbf{0.09}$	$32^3 \times 96$	0.15	≈ 0.045	$64^3 \times 192$	0.2

Table 1: Summary of all ensembles to be included in the full analysis. The ensembles in bold have been analyzed for this report. Light(strange) sea quark masses are denoted by $m_l(m_h)$.

3. Results

We report on results from an analysis of a large set of gauge field ensembles generated in the presence of $2+1$ flavors of improved staggered (asqtad) quarks [14, 15]. Further ensembles will be included in the future. Some key ensemble parameters are listed in Table 3.

On each ensemble we compute the three-point correlation functions relevant to the weak matrix elements and the two-point functions relevant to the propagation of the B and D mesons. For the heavy-light mesons we use heavy clover quarks in the Fermilab interpretation and light, improved staggered (asqtad) quarks [14, 15]. We use two types of interpolating operators for the B and D mesons, namely local and smeared using the 1S Richardson wave function. We set the valence-quark masses equal to the sea-quark masses. The bare lattice charm and bottom quark masses are fixed by matching the kinetic masses of the D_s and B_s mesons, respectively, to their experimental values. Some small adjustments will be needed to refine this tuning but are not yet included in this preliminary analysis.

In terms of interpolating operators $\mathcal{O}_B$ and $\mathcal{O}_D$ for the B and D mesons and the vector current, the two-point and three-point functions are given by

$$C^{2pt}(t; \mathbf{p}) = \sum_{\mathbf{x}} \exp(i\mathbf{p} \cdot \mathbf{x}) \langle \mathcal{O}(\mathbf{x}, t) \mathcal{O}^\dagger(\mathbf{0}) \rangle$$

$$= \sum_n s_n^t Z_n(\mathbf{p}) [\exp(-E_n(\mathbf{p})t) + \exp(-E_n(\mathbf{p})(N_t - t))] \quad (3.1)$$

$$C_{V_\mu}^{3pt, B \rightarrow D}(t, T; \mathbf{p}) = \sum_{\mathbf{x}, \mathbf{y}} \exp(i\mathbf{p} \cdot \mathbf{y}) \langle \mathcal{O}_D(0) V_\mu(\mathbf{y}, t) \mathcal{O}_B^\dagger(\mathbf{x}, T) \rangle, \quad (3.2)$$

where $s_n = \pm 1$ accounts for contributions that oscillate in t , and N_t is the lattice extent in the t dimension. Note that in the three-point function above, we have put the D meson at the origin and the B meson at $(\mathbf{x}, T)$.

The matrix elements we want from Eq. (2.6) to Eq. (2.8) are obtained by factorization and reduction of the three-point functions. The reduction is based on the overlap coefficients $Z_n(\mathbf{p})$, energies and masses obtained in fits to the two-point functions. For example, the $R_+(\mathbf{p})$ matrix element is obtained from

$$R_+(t, T; \mathbf{p}) = \frac{C_{V_4}^{3pt, B \rightarrow D}(t, T; \mathbf{p})}{\sqrt{C_{V_4}^{3pt, D \rightarrow D}(t, T; \mathbf{0}) C_{V_4}^{3pt, B \rightarrow B}(t, T; \mathbf{0})}} \sqrt{\frac{Z_D(\mathbf{0}) E_D}{Z_D(\mathbf{p}) m_D}} e^{E_D t - \frac{1}{2} m_D T} e^{-m_B(t - \frac{1}{2} T)} \quad (3.3)$$

in the limit $t \rightarrow \infty$ and $T - t \rightarrow \infty$. In that limit it is a constant, $R_+(\mathbf{p})$, independent of t . However, at finite t and T , complications from oscillating terms and excited states must be taken into account.

Because they contain a light staggered quark, the meson interpolating operators excite even- as well as odd-parity channels. The unwanted even-parity states manifest themselves as terms that oscillate in t , corresponding to terms in the two-point and three-point functions with $s_n = -1$. To suppress the effect of the oscillating terms in the three-point functions, we average in both t and T (after removing the dominant exponential dependence on t as in Eq. (3.3)) as follows:

$$\bar{R} \equiv \frac{1}{2}R(0, t, T) + \frac{1}{4}R(0, t, T+1) + \frac{1}{4}R(0, t+1, T+1). \quad (3.4)$$

Here, R refers to any of the quantities derived from three-point functions, such as R_+ , R_- , and x_f .

Having suppressed the contributions of the oscillating states to the three-point correlators, we must still account for contributions from excited states. For example, for $D \rightarrow D$, the leading contributions are

$$\begin{aligned} C_{V4}^{3ptD \rightarrow D}(p, t) = & \sqrt{Z_D(p)} \frac{e^{-E_D t}}{\sqrt{2E_D}} \langle D | V_4 | D \rangle \frac{e^{-m_D(T-t)}}{\sqrt{2m_D}} \sqrt{Z_D(0)} + \sqrt{Z_{D'}(p)} \frac{e^{-E_{D'} t}}{\sqrt{2E_{D'}}} \\ & \times \langle D' | V_4 | D \rangle \frac{e^{-m_D(T-t)}}{\sqrt{2m_D}} \sqrt{Z_D(0)} + \sqrt{Z_D(p)} \frac{e^{-E_D t}}{\sqrt{2E_D}} \langle D | V_4 | D' \rangle \frac{e^{-m_{D'}(T-t)}}{\sqrt{2m_{D'}}} \sqrt{Z_{D'}(0)}, \end{aligned} \quad (3.5)$$

where the primes indicate the overlaps and energies of the excited states of the same parity. We have neglected the doubly excited contribution, since the singly excited contribution is found already to be small. Thus, at finite t and T the ratio $R_+(t, T; \mathbf{p})$ in Eq. (3.3) is not constant, but has a small contamination from excited states. We take this into account by fitting the resulting ratio to

$$R_+(\mathbf{p}, t, T) = R_+(\mathbf{p}) \exp(\delta m t) + A \exp(-\Delta E_D t) + B \exp(-\Delta m_B (T - t)) \quad (3.6)$$

as illustrated in Fig. 2. The fit parameter δm should be zero, but it is introduced to allow for a small error in determining E_D and m_B . The other terms involve $\Delta E_D = E_{D'} - E_D$ and $\Delta m_B = m_{B'} - m_B$. These parameters are obtained from the fits of two-point functions. The results of two-point function fits then become prior central values and widths for fitting $R_+(t, T; \mathbf{p})$. We use a similar method to obtain $R_-(\mathbf{p})$ and $x_f(\mathbf{p})$.

4. Chiral and continuum extrapolation

To complete the analysis we will extrapolate in the light quark masses to their physical values and take the continuum limit, using staggered chiral perturbation theory [16, 17]. At this preliminary stage, we don't show physical values and chiral fit in this report. The numerical data points for h_+ and h_- are shown in Fig. 3. We will need these data points to finish the extrapolation of physical value of h_+ and h_- and the chiral fit.

5. Future plans

To complete the project, we need to (1) finish analyzing the available ensembles, (2) make adjustments for the tuning of the heavy quark masses, (3) compute the current renormalization (ρ_V factor), and (4) combine the experimental results for the differential decay rate with our results for the form factor to obtain $|V_{cb}|$, using methods employed for $|V_{ub}|$ to extend w over the full kinematic range [18].

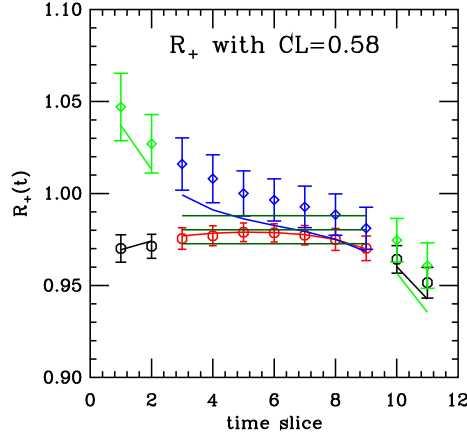


Figure 2: A sample fit to $R_+(t, T; \mathbf{p})$. Example three-point correlation fit for the 0.12 fm 0.14 m_l/m_h ensemble. The circles correspond to the local source, and diamonds, the smeared source. The fit result is obtained by a simultaneous fit to both correlators using Eq. (3.3). The horizontal lines represent the central value and error of the result for $R_+(\mathbf{p})$.

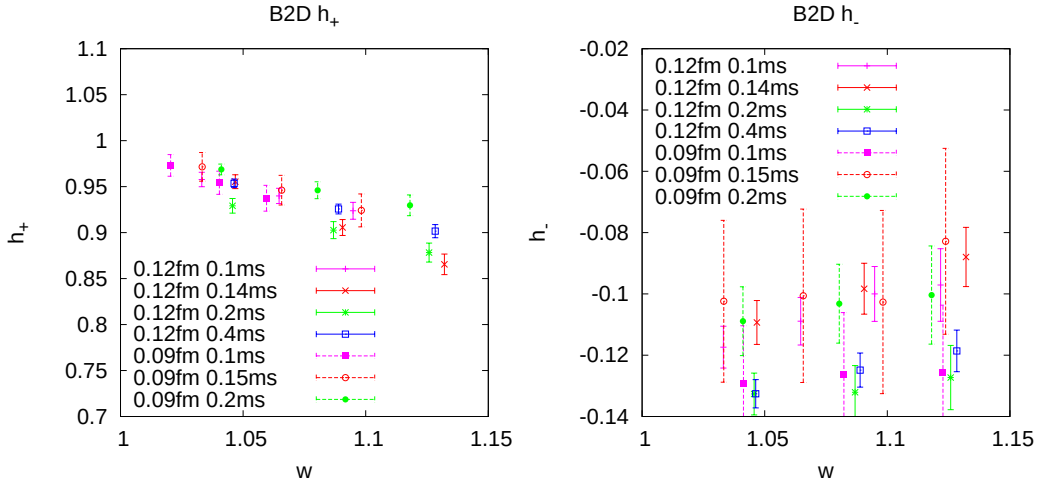


Figure 3: Form factors h_+ (left) and h_- (right) vs. w , omitting the matching factor ρ_V , on the bold ensembles in Table 3. The color code is given in the legends.

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References

- [1] C. G. Boyd, Z. Ligeti, I. Z. Rothstein, and M. B. Wise, Phys. Rev. D **55** (1997) 3027 [arXiv:hep-ph/9610518].
- [2] S. Hashimoto, A. S. Kronfeld, P. B. Mackenzie, S. M. Ryan, and J. N. Simone, Phys. Rev. D **66** (2002) 014503 [hep-ph/0110253].
- [3] C. Bernard *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. D **79** (2009) 014506 [arXiv:0808.2519 [hep-lat]].
- [4] J. A. Bailey *et al.* [Fermilab Lattice and MILC Collaborations], PoS **LATTICE2010** (2010) 311 [arXiv:1011.2166 [hep-lat]].
- [5] P. B. Mackenzie, talk at Workshop on CKM Unitarity Triangle, Warwick, UK (September 2010).
- [6] A. S. Kronfeld, Phys. Rev. D **62** (2000) 014505 [hep-lat/0002008].
- [7] J. Harada, S. Hashimoto, A. S. Kronfeld, and T. Onogi, Phys. Rev. D **65** (2002) 094514 [hep-lat/0112045].
- [8] G. M. de Divitiis, E. Molinaro, R. Petronzio, N. Tantalo, Phys. Lett. B **655** (2007) 45 [arXiv:0707.0582 [hep-lat]].
- [9] J. Laiho, E. Lunghi, and R. S. Van de Water, Phys. Rev. D **81** (2010) 034503 [arXiv:0910.2928 [hep-ph]].
- [10] J. Laiho, E. Lunghi, and R. S. Van de Water, <http://latticeaverages.org/>, accessed July, 2011.
- [11] Heavy Flavor Averaging Group, <http://www.slac.stanford.edu/xorg/hfag/semi/>, accessed July, 2011.
- [12] J. E. Bartelt *et al.* [CLEO Collaboration], Phys. Rev. Lett. **82** (1999) 3746 [hep-ex/9811042].
- [13] A. X. El-Khadra, A. S. Kronfeld, P. B. Mackenzie, Phys. Rev. D **55** (1997) 3933 [hep-lat/9604004].
- [14] C. W. Bernard *et al.* [MILC Collaboration], Phys. Rev. D **61** (2000) 111502 [hep-lat/9912018].
- [15] A. Bazavov *et al.*, Rev. Mod. Phys. **82** (2010) 1349 [arXiv:0903.3598 [hep-lat]].
- [16] C. K. Chow and M. B. Wise, Phys. Rev. D **48** (1993) 5202 [arXiv:hep-ph/9305229].
- [17] J. Laiho and R. S. Van de Water, Phys. Rev. D **73** (2006) 054501 [hep-lat/0512007].
- [18] J. A. Bailey *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. D **79** (2009) 054507 [arXiv:0811.3640 [hep-lat]].

Semileptonic form factor ratio $B_s \rightarrow D_s/B \rightarrow D$ and its application to $BR(B_s^0 \rightarrow \mu^+ \mu^-)$

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We present a (2+1)-flavor lattice QCD calculation of the form factor ratio between the semileptonic decays $\bar{B}_s^0 \rightarrow D_s^+ l^- \bar{\nu}$ and $\bar{B}^0 \rightarrow D^+ l^- \bar{\nu}$. This ratio is an important theoretical input to the hadronic determination of the B meson fragmentation fraction ratio f_s/f_d which enters in the measurement of $BR(B_s^0 \rightarrow \mu^+ \mu^-)$. Small lattice spacings and high statistics enable us to simulate the decays with a dynamic final D meson of small momentum and reliably extract the hadronic matrix elements at nonzero recoil. We report our preliminary result for the form factor ratio at the corresponding momentum transfer of the two decays $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$.

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1. Introduction

The rare decay $B_s^0 \rightarrow \mu^+ \mu^-$ is a process that is potentially sensitive to physics beyond the standard model (SM). In the SM, the decay can go only through penguin or box topologies at the loop level. Thus, a small branching fraction has been predicted, with the aid of lattice QCD, to be $3.2(2) \times 10^{-9}$ [1, 2]. Recently, LHCb [3] and CDF [4] reported bounds on the branching fraction, to be followed by upcoming results from CMS. It is likely that a 5σ measurement will be made, even at the SM branching ratio, in the near future.

At LHCb, the extraction of the branching fraction relies on the normalization channels $B_u^+ \rightarrow J/\psi K^+$, $B_d^0 \rightarrow K^+ \pi^-$ and $B_s^0 \rightarrow J/\psi \phi$ [5], through the following relation

$$\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-) = \text{BR}(B_q \rightarrow X) \frac{f_q}{f_s} \frac{\varepsilon_X}{\varepsilon_{\mu\mu}} \frac{N_{\mu\mu}}{N_X}, \quad (1.1)$$

where ε and N are the detector efficiencies and number of events. The fragmentation fractions, f_q ($q = u, d, s$ or Λ), denote the probability of a b quark hadronizing into a B_q meson or a b -flavored (e.g., Λ_b) baryon. The fragmentation fraction ratio f_s/f_d is crucial in the extraction of $\text{BR}(B_s^0 \rightarrow \mu^+ \mu^-)$. Currently, the uncertainty in f_s/f_d is the major source of uncertainty. Traditionally, f_s/f_d was measured using the ratio of the corresponding semileptonic decays. Fleischer, Serra and Tuning proposed [6] that the ratio can also be measured using the non-leptonic decays $\bar{B}_s^0 \rightarrow D_s^+ \pi^-$ and $\bar{B}_d^0 \rightarrow D^+ K^-$, which has the advantages of a cleaner background, similar reconstruction of final states, etc. The approach is based on factorization of the nonleptonic amplitudes into f_π or f_K and corresponding semileptonic form factors. The ratio f_s/f_d is related to $\text{BR}(\bar{B}_s \rightarrow D\pi)/\text{BR}(\bar{B} \rightarrow DK)$ in a way similar to Eq. (1.1). With the efficiencies and event counts combined with the factorization approximation, we have

$$\frac{f_s}{f_d} = \frac{|V_{us}|^2 f_K^2}{|V_{ud}|^2 f_\pi^2} \times \frac{\tau_{B^0}}{\tau_{B_s^0}} \times \left[\frac{\varepsilon_{DK}}{\varepsilon_{D_s\pi}} \frac{N_{D_s\pi}}{N_{DK}} \right] \times \frac{1}{\mathcal{N}_a \mathcal{N}_F}, \quad (1.2)$$

where τ is the lifetime and $\mathcal{N}_a \approx 1$ with corrections of a few percent due to nonfactorizable effects [6]. The semileptonic form factor ratio $\mathcal{N}_F = [f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)]^2$ is currently the decisive contributor to the theoretical error. The value currently used at LHCb is an estimate from QCD sum rules, $\mathcal{N}_F = 1.24(8)$ [7, 6]. However, this theoretical input and the size of its error need to be validated by a nonperturbative method such as lattice QCD. This paper is devoted to such a calculation.

The matrix elements of the $B \rightarrow D$ semileptonic decay (and similarly for $B_s \rightarrow D_s$) can be written as

$$\langle D(p') | \mathcal{V}^\mu | B(p) \rangle = f_+(q^2) \left[(p + p')^\mu - \frac{M_B^2 - M_D^2}{q^2} q^\mu \right] + f_0(q^2) \frac{M_B^2 - M_D^2}{q^2} q^\mu. \quad (1.3)$$

However, for heavy quarks it is convenient to use the variables $h_\pm$, defined by

$$\frac{\langle D(p') | \mathcal{V}^\mu | B(p) \rangle}{\sqrt{M_B M_D}} = h_+(w) (v + v')^\mu + h_-(w) (v - v')^\mu, \quad (1.4)$$

where $v = p/M$ and the recoil variable is $w = v \cdot v'$. We will use the form factors $h_\pm$ in our entire analysis and convert them in the end to f_+ , f_0 using Eqs. (1.3) and (1.4).

In these proceedings, we report a preliminary result of the form factor ratio $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$ by analyzing the semileptonic decays $\bar{B}_s^0 \rightarrow D_s^+ l^- \bar{\nu}$ and $\bar{B}^0 \rightarrow D^+ l^- \bar{\nu}$ on the lattice. We use an

identical subset of the MILC gauge configurations for both of the $B_s \rightarrow D_s$ and $B \rightarrow D$ processes. To reduce the statistical errors effectively, we construct a set of ratios at small recoil, from which we extract the lattice form factors $h_{\pm}$. The extrapolation to physical light quark masses and to the continuum is performed using root staggered chiral perturbation theory (rS χ PT). The results are extrapolated to maximum recoil by employing a model-independent parametrization. In Sec.4, we report our lattice result.

2. Numerical details

2.1 Data setup

Our calculation uses four ensembles of the MILC's (2+1)-flavor gauge configurations [8], two at each of the lattice spacings $a \approx 0.12$ fm and ≈ 0.09 fm. The ensembles as well as the parameters used are summarized in Table 1. The strange and light sea quarks were simulated using the asqtad-improved staggered action [9]. The action is also used in our strange and light valence quarks. The heavy quarks (charm and bottom) are simulated using the Sheikholeslami-Wohlert (SW) clover action with the Fermilab interpretation [10]. For the $B \rightarrow D$ decay, the spectator light quark is degenerate with the light sea quark (full QCD). While for the $B_s \rightarrow D_s$ decay, the strange quark is set close to its physical value. The charm and bottom quarks in our calculation are tuned to their physical values up to a tuning uncertainty. The corresponding bare hopping parameter $\kappa_{b(c)}$, as well as the coefficient for the clover term c_{SW} are given explicitly in Table 1.

2.2 Lattice extraction

In this work, we are interested only in the vector current operator. On the lattice we define $V^\mu = \sqrt{Z_{V4}^{cc} Z_{V4}^{bb}} \bar{\Psi}_c i\gamma^\mu \Psi_b$, where Z^{hh} are normalization factors. The vector current in the continuum is $\mathcal{V}^\mu = \rho_{V\mu} V^\mu$, where $\rho_{V\mu}^2 = Z_{V\mu}^{bc} Z_{V\mu}^{cb} / Z_{V4}^{bb} Z_{V4}^{cc}$. The factor $\rho_{V\mu}$ can be calculated perturbatively and has been found to be very close to one [11, 12]. We expect the ρ_V s to largely cancel in the ratio of the form factors. Hence this correction is negligible compared with other systematic errors and we take $\rho_V = 1$ for this analysis.

We employ the following three-point functions in our analysis,

$$C_{3pt}^{DV^\mu B}(0, t, T; \mathbf{p}_D) = \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \mathcal{O}_D(0, \mathbf{0}) \bar{\Psi}_c i\gamma^\mu \Psi_b(t, \mathbf{y}) \mathcal{O}_B^+(0, \mathbf{x}) | 0 \rangle e^{i\mathbf{p}_D \cdot \mathbf{y}}, \quad (2.1)$$

$$C_{3pt}^{DV^\mu D}(0, t, T; \mathbf{p}_D) = \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \mathcal{O}_D(0, \mathbf{0}) \bar{\Psi}_c i\gamma^\mu \Psi_c(t, \mathbf{y}) \mathcal{O}_D^+(0, \mathbf{x}) | 0 \rangle e^{i\mathbf{p}_D \cdot \mathbf{y}}, \quad (2.2)$$

$$C_{3pt}^{BV^4 B}(0, t, T; \mathbf{0}) = \sum_{\mathbf{x}, \mathbf{y}} \langle 0 | \mathcal{O}_B(0, \mathbf{0}) \bar{\Psi}_b i\gamma^4 \Psi_b(t, \mathbf{y}) \mathcal{O}_B^+(0, \mathbf{x}) | 0 \rangle. \quad (2.3)$$

The B meson is at rest. To obtain the dependence of the form factors at small recoil w , we simulate the final state D meson at a few small momenta, i.e., $\mathbf{p} = 2\pi(1, 0, 0)/L$, $2\pi(1, 1, 0)/L$, $2\pi(1, 1, 1)/L$

a (fm)	am_l/am_s	N_{confs}	c_{SW}	κ_c	κ_b	$am_x(B \rightarrow D)$	$am_x(B_s \rightarrow D_s)$
≈ 0.12	0.020/0.050	2052	1.525	0.1259	0.0918	0.020	0.0349
≈ 0.12	0.007/0.050	2110	1.530	0.1254	0.0901	0.007	0.0349
≈ 0.09	0.0124/0.031	1996	1.473	0.1277	0.0982	0.0124	0.0261
≈ 0.09	0.0062/0.031	1931	1.476	0.1276	0.0979	0.0062	0.0261

Table 1: MILC ensembles of configurations used in this analysis.

and $2\pi(2,0,0)/L$. The correlation functions for $D \rightarrow D$ and $B \rightarrow B$ serve as normalization. The $D \rightarrow D$ correlation function with a non-zero final state momentum is used to extract the recoil w to alleviate the need of renormalizing the four velocity.

From these correlation functions we construct three different ratios, fits to which include contributions from the lowest-order excited states. Explicitly,

$$\frac{C_{3pt}^{DV^iD}(0,t,T;\mathbf{p})}{C_{3pt}^{DV^4D}(0,t,T;\mathbf{p})} = d^i (1 + \mathcal{D}_{02} e^{-\Delta E(\mathbf{0})(T-t)} + \mathcal{D}_{20} e^{-\Delta E(\mathbf{p})t}), \quad (2.4)$$

$$\frac{C_{3pt}^{DV^iB}(0,t,T;\mathbf{p})}{C_{3pt}^{DV^4B}(0,t,T;\mathbf{p})} = b^i (1 + \mathcal{B}_{02} e^{-\Delta m(T-t)} + \mathcal{B}_{20} e^{-\Delta E(\mathbf{p})t}), \quad (2.5)$$

$$\begin{aligned} \frac{C_{3pt}^{DV^iB}(0,t,T;\mathbf{p})}{C_{3pt}^{DV^4B}(0,t,T;\mathbf{0})} &\times \left[\frac{Z_0(\mathbf{0})}{Z_0(\mathbf{p})} \sqrt{\frac{E_0(\mathbf{p})}{E_0(\mathbf{0})}} e^{(E_0(\mathbf{p})-E_0(\mathbf{0}))t} \right] \\ &= a^i (1 + \mathcal{A}_{02} e^{-\Delta m(T-t)} + \mathcal{A}_{20} e^{-\Delta E(\mathbf{p})t} + \mathcal{A}'_{20} e^{-\Delta E_2(\mathbf{0})t}) e^{\delta t}. \end{aligned} \quad (2.6)$$

The factor in the square brackets of Eq. (2.6) cancels the time dependence of the ratio, stemming from the fact that the numerator and denominator have final state D mesons with different momenta. ΔE and Δm denote the lowest splittings and δ is a parameter that accounts for the imprecise $E(\mathbf{p}) - E(\mathbf{0})$ in the bracket in Eq. (2.6). In the fits the lowest-lying energy splittings ΔE , Δm are treated as fit parameters. The splittings can be extracted from the two-point functions. So, we employ a multi-channel fitting procedure, combining the two-point functions and the ratios of the three-point functions. We find that such a treatment results in more robust fits and more precise splittings. From d_i, b_i and a_i we can easily recover the form factors $h_{\pm}$ at small recoil w ,

$$w = \frac{1 + \mathbf{d} \cdot \mathbf{d}}{1 - \mathbf{d} \cdot \mathbf{d}}, \quad (2.7)$$

$$h_+(w) = h_+(1)(a_i/b_i - \mathbf{a} \cdot \mathbf{d}), \quad (2.8)$$

$$h_-(w) = h_+(1)(a_i/b_i - a_i/d_i). \quad (2.9)$$

3. Results

The extrapolation of our lattice results to the physical quark masses and the continuum is guided by rS χ PT [13, 14]. However, in the case of h_+ the light quark mass dependence is accompanied by a small recoil w dependence. Such a dependence was included in the continuum chiral perturbation theory in Ref. [15] and was extended to the NLO rS χ PT in Ref. [16]. For h_- , the NLO correction is simply a constant which is inversely proportional to the charm quark mass. We follow the same setup, adding NNLO analytic terms and including a^2 dependence. The remaining recoil dependence of the form factors is fitted to a simple quadratic expansion at zero recoil.

The results of the chiral/continuum extrapolation are shown in Fig. 1. The form factor h_+ for both of the $B \rightarrow D$ and $B_s \rightarrow D_s$ decays shows a small dependence on the light quark masses and lattice spacings. The extrapolated physical values are very close to the lattice data points. This suggests that h_+ is insensitive to the light degrees of freedom. However, sizable light quark mass and lattice spacing dependence appears in the case of h_- , as indicated by the variation due to the sea quark masses and the differences between $h_-^{B \rightarrow D}$ and $h_-^{B_s \rightarrow D_s}$ (spectator mass). Note that the difference between $h_+^{B \rightarrow D}$ and $h_+^{B_s \rightarrow D_s}$ is minor. Considering the subleading role that h_- plays in contributing to f_+ , f_0 , we expect the U-spin symmetry breaking effect to be smaller than what was

expected in [6, 7]. Such an observation is bolstered by the recent lattice calculations on f_+, f_0 of the $D_{(s)} \rightarrow \pi(K)$ decays [17].

With the physical values of $h_{\pm}$, we can easily calculate f_0, f_+ using the physical masses of the D and B mesons. However, to evaluate the form factors at a small momentum transfer ($q^2 = M_{\pi}^2, M_K^2$), we need to extrapolate the results near maximum recoil. We use the model-independent z -parametrization [18] with the constraint $f_0(0) = f_+(0)$. We take four synthetic points in the recoil range where we have lattice data points. We take the values of f_+, f_0 by evaluating our chiral/continuum extrapolation result at these four recoil points and perform the z -parametrization. The result is shown in Figure 2. We study the effect of a pole at a vector B_c meson in the Blasck factor of the z -expansion of f_+ . We find that the shapes of the form factors are only weakly affected by the inclusion of such a pole.

By expanding the form factors at the respective momentum transfers, we finally arrive at

$$f_0^{(s)}(M_{\pi}^2)/f_0^{(d)}(M_K^2) = 1.051(40)(22). \quad (3.1)$$

The first error is from statistics. The second error is the systematical error due only to the uncertainty on $g_{DD^*\pi}$ and to the variation of fits in the z -parametrization. We are in the process of building a full systematic error budget.

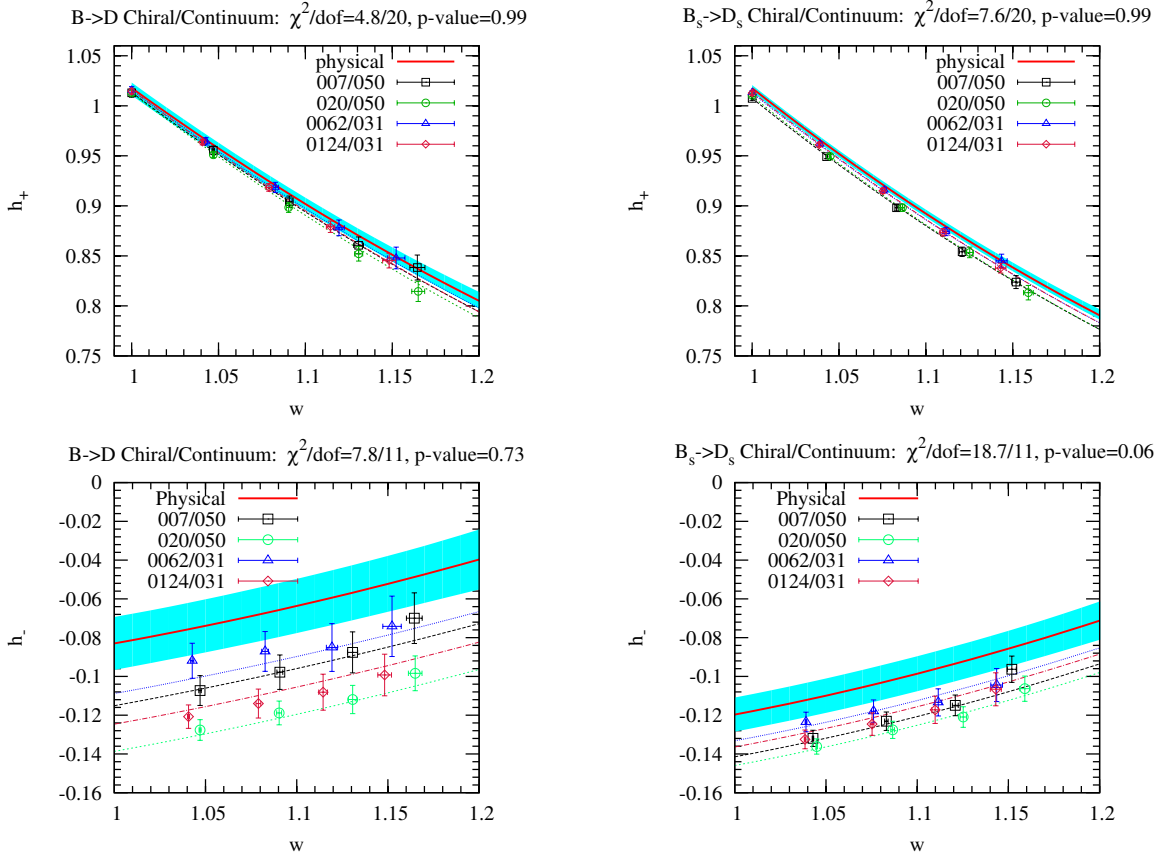


Figure 1: Chiral/continuum extrapolation of $h_{\pm}(w)$ for the $B \rightarrow D$ (left) and $B_s \rightarrow D_s$ decays (right).

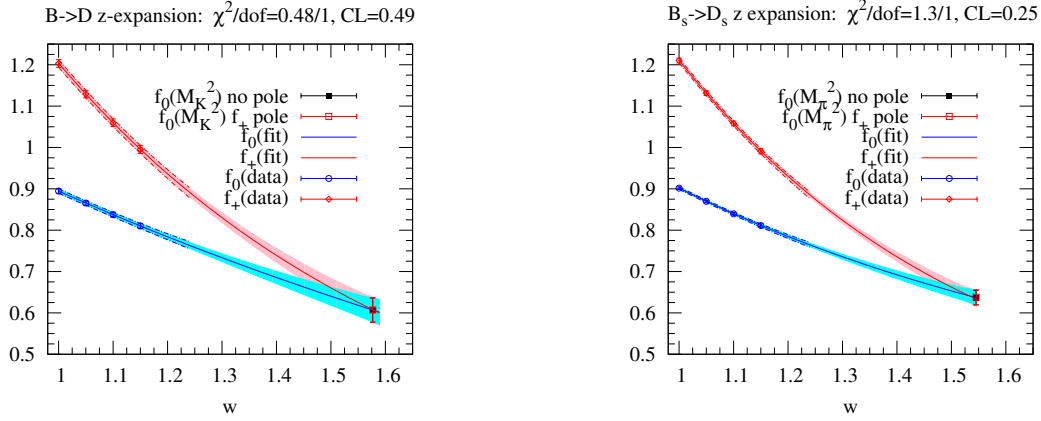


Figure 2: The z -expansion of form factors f_0, f_+ . The points that we include in the z -expansion fits are shown explicitly. The dashed curves indicate the result of chiral/continuum extrapolation.

4. Conclusions

In summary, we present a (2+1)-flavor lattice QCD calculation of the form factor ratio $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2)$, which is a major theoretical input for the extraction of the fragmentation fraction ratio f_s/f_d . The essential part of our calculation is to extract the $B \rightarrow D$ and $B_s \rightarrow D_s$ semileptonic form factors at non-zero recoil. We reduce the systematic uncertainty by fitting the lowest-order excited states, and we employ a simultaneous multi-channel fit procedure to address correlations and reduce the statistical uncertainty. Our chiral/continuum results show that the corrections to the finite lattice spacings and finite light quark masses are small. Our preliminary result is $f_0^{(s)}(M_\pi^2)/f_0^{(d)}(M_K^2) = 1.051(40)(22)$, with a partial systematic error budget. As a consequence, we obtain $\mathcal{N}_F = 1.105(80)(44)$ which implies a smaller U-spin breaking effect than that suggested in [7], $\mathcal{N}_F = 1.24(8)$. A more comprehensive analysis with a detailed error budget is still in progress and will be reported in a forthcoming paper.

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References

- [1] **HPQCD** Collaboration, E. Gámiz, C. T. H. Davies, G. P. Lepage, J. Shigemitsu, and M. Wingate, *Neutral B meson mixing in unquenched lattice QCD*, *Phys. Rev.* **D80** (2009) 014503 [arXiv:0902.1815 [hep-lat]]
- [2] A. J. Buras, *Relations between $\Delta M_{s,d}$ and $B_{s,d} \rightarrow \mu\bar{\mu}$ in models with minimal flavor violation*, *Phys. Lett.* **B566** (2003) 115–119 [hep-ph/0303060]
- [3] **LHCb** Collaboration, R. Aaij *et al.*, *Search for the rare decays $B_s \rightarrow \mu\mu$ and $B_d \rightarrow \mu\mu$* , *Phys. Lett.* **B699** (2011) 330–340 [arXiv:1103.2465 [hep-ex]]
- [4] **CDF** Collaboration, T. Aaltonen *et al.*, *Search for $B_s \rightarrow \mu^+\mu^-$ and $B_d \rightarrow \mu^+\mu^-$ Decays with CDF II*, arXiv:1107.2304 [hep-ex]
- [5] **LHCb** Collaboration, B. Adeva *et al.*, *Roadmap for selected key measurements of LHCb*, arXiv:0912.4179 [hep-ex]
- [6] R. Fleischer, N. Serra, and N. Tuning, *A new strategy for B_s branching ratio measurements and the search for new physics in $B_s^0 \rightarrow \mu^+\mu^-$* , *Phys. Rev.* **D82** (2010) 034038 [arXiv:1004.3982 [hep-ph]]
- [7] P. Blasi, P. Colangelo, G. Nardulli, and N. Paver, *Phenomenology of B_s decays*, *Phys. Rev.* **D49** (1994) 238–246 [hep-ph/9307290]
- [8] A. Bazavov *et al.*, *Nonperturbative QCD simulations with 2+1 flavors of improved staggered quarks*, *Rev. Mod. Phys.* **82** (2010) 1349–1417 [arXiv:0903.3598 [hep-lat]]
- [9] G. Lepage, *Flavor symmetry restoration and Symanzik improvement for staggered quarks*, *Phys. Rev.* **D59** (1999) 074502 [hep-lat/9809157]
- [10] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, *Massive fermions in lattice gauge theory*, *Phys. Rev.* **D55** (1997) 3933–3957 [hep-lat/9604004]
- [11] A. S. Kronfeld, *Application of heavy quark effective theory to lattice QCD I: Power corrections*, *Phys. Rev.* **D62** (2000) 014505 [hep-lat/0002008]
- [12] J. Harada, S. Hashimoto, A. S. Kronfeld, and T. Onogi, *Application of heavy quark effective theory to lattice QCD III: Radiative corrections to heavy-heavy currents*, *Phys. Rev.* **D65** (2002) 094514 [hep-lat/0112045]
- [13] C. Aubin and C. Bernard, *Pion and kaon masses in staggered chiral perturbation theory*, *Phys. Rev.* **D68** (2003) 034014 [hep-lat/0304014]
- [14] J. Laiho and R. S. Van de Water, *$B \rightarrow D^*\ell\nu$ and $B \rightarrow D\ell\nu$ form factors in staggered chiral perturbation theory*, *Phys. Rev.* **D73** (2006) 054501 [hep-lat/0512007]
- [15] C.-K. Chow and M. B. Wise, *Corrections from low momentum physics to heavy quark symmetry relations for $B \rightarrow D\ell\bar{\nu}_e$ and $B \rightarrow D^*\ell\bar{\nu}_e$ decay*, *Phys. Rev.* **D48** (1993) 5202–5207 [hep-ph/9305229]
- [16] J. Laiho, unpublished notes, 2010
- [17] **HPQCD** Collaboration, J. Koponen *et al.*, *The D to K and D to pi semileptonic decay form factors from Lattice QCD*, [arXiv:1111.0225 [hep-lat]]
- [18] C. Boyd, B. Grinstein, and R. F. Lebed, *Constraints on form-factors for exclusive semileptonic heavy to light meson decays*, *Phys. Rev. Lett.* **74** (1995) 4603–4606 [hep-ph/9412324]

Calculation of $K \rightarrow \pi l \nu$ form factors with $N_f = 2 + 1$ flavours of staggered quarks

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We report on the status of the Fermilab-MILC calculation of the form factor $f_+^{K\pi}(q^2 = 0)$, needed to extract the CKM matrix element $|V_{us}|$ from experimental data on K semileptonic decays. The HISQ formulation is used in the simulations for the valence quarks, while the sea quarks are simulated with the asqtad action (MILC $N_f = 2 + 1$ configurations). We discuss the general methodology of the calculation, including the use of twisted boundary conditions to get values of the momentum transfer close to zero and the different techniques applied for the correlators fits. We present initial results for lattice spacings $a \approx 0.12$ fm and $a \approx 0.09$ fm, and several choices of the light quark masses.

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1. Introduction

The error associated with the lattice determination of the form factor $f_+^{K\pi}(0)$ ($\sim 0.5\%$) is still the dominant uncertainty in the extraction of $|V_{us}|$ from experimental data on K semileptonic decays: $|V_{us}| f_+^{K\pi}(0) = 0.2163(\pm 0.23\%)$ [1]. Improvement in the determination of that form factor is thus crucial in order to extract all the information from the available experimental data.

A precise value of $|V_{us}|$ is needed to check unitarity in the first row of the CKM matrix. Any deviation from unitarity would indicate the existence of beyond the Standard Model physics. But, even if unitarity is fulfilled, however, as it is the case with current experimental and theoretical inputs, this test can establish very stringent constraints on the scale of the allowed new physics (~ 10 TeV) [1]. One also could compare the values of $|V_{us}|$ as extracted from helicity-allowed semileptonic decays and helicity-suppressed leptonic decays in the search for deviations from SM predictions. In particular, it is useful to study the ratio

$$R_{\mu 23} = \left(\frac{f_+^{K\pi}(0)}{f_K/f_\pi} \right)_{\text{lattice}} \left(\left| \frac{V_{us}}{V_{ud}} \right| \frac{f_K}{f_\pi} \right)_{\mu 2} \frac{|V_{ud}|}{[|V_{us}| f_+^{K\pi}(0)]_{l3}}, \quad (1.1)$$

where the subscripts $\mu 2$ and $l3$ indicate that those quantities are obtained from experimental data on leptonic $K_{\mu 2}$ and semileptonic K_{l3} decays respectively. The ratio in (1.1) is unity in the SM but not in some extensions of the SM, for example, those with a charged Higgs. Again, the error in the current value $R_{\mu 23} = 0.999(7)$ [1] is limited by the precision of lattice-QCD inputs.

In these proceedings we report on the status of the calculation of the form factor $f_+^{K\pi}(0)$ using staggered quarks. The goal of this analysis is to show that the staggered formulation can provide a determination of this parameter competitive with the state of the art unquenched determinations [3] by addressing the main sources of systematic errors and improving in statistics.

2. Methodology: extracting the form factor directly at $q^2 = 0$

Semileptonic K decays are parametrized in terms of the form factors f_+ and f_0 in the following way

$$\langle \pi | V^\mu | K \rangle = f_+^{K\pi}(q^2) \left[p_K^\mu + p_\pi^\mu - \frac{m_K^2 - m_\pi^2}{q^2} q^\mu \right] + f_0^{K\pi}(q^2) \frac{m_K^2 - m_\pi^2}{q^2} q^\mu, \quad (2.1)$$

where $q = p_K - p_\pi$ and V^μ is the appropriate flavour changing vector current. One of the main components of our analysis which reduces both systematic and statistical errors is the use of the method developed by the HPQCD collaboration to study charm semileptonic decays [2]. This method is based on the Ward identity relating the matrix element of a vector current to that of the corresponding scalar current: $q^\mu \langle \pi | V_\mu^{lat} | K \rangle Z = (m_s - m_q) \langle \pi | S^{lat} | K \rangle$, with $S = \bar{s}l$, and Z a lattice renormalization factor for the vector current. In this work, we use the local scalar density of staggered fermions, so the combination $(m_s - m_q)S$ requires no renormalization. Using the definition of the form factors in Eq. (2.1) and this identity, one can extract $f_0^{K\pi}(q^2)$ at any q^2 by using

$$f_0^{K\pi}(q^2) = \frac{m_s - m_l}{m_K^2 - m_\pi^2} \langle \pi | S | K \rangle (q^2). \quad (2.2)$$

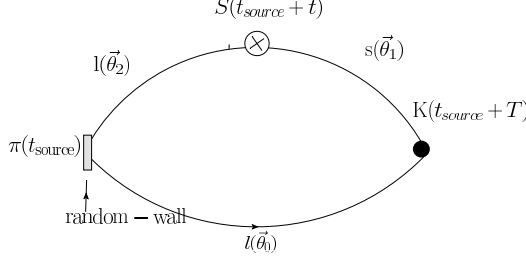


Figure 1: Structure of the 3-point functions needed to calculate $f_0^{K\pi}(q^2)$. Light-quark propagators are generated at t_{source} with random-wall sources. An extended strange propagator is generated at T .

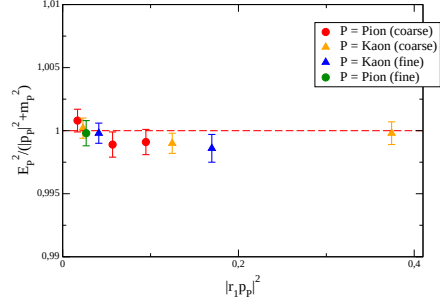


Figure 2: Deviation of our data from the continuum dispersion relation prediction.

Kinematic constraints demand that $f_+(0) = f_0(0)$, so this relation can be used to calculate $f_+^{K\pi}(0)$. One of the main advantages of relation (2.2) is that it avoids the use of a renormalization factor to obtain the form factor f_0 . The drawback to this method is that it gives no access to the shape of $f_+^{K\pi}$, but in this analysis we are focusing on the extraction of $|V_{us}|$, so we need the normalization of the form factor only at a single point.

Another key ingredient is employing twisted boundary conditions [5, 6] to simulate the relevant correlations functions directly at $q^2 = 0$. This avoids an interpolation in q^2 and thus the corresponding systematic uncertainty. In Fig. 1 we plot the general structure of the relevant 3-point functions. In order to get $q^2 = 0$, we inject momentum $\vec{p} = \vec{\theta}\pi/L$ in either the kaon or the pion. For a non-zero $\vec{p}_K$ we chose $\vec{\theta}_0 = \vec{\theta}_2 = 0$, $\vec{\theta}_1 \neq \vec{0}$, and for a non-zero $\vec{p}_\pi$ we chose $\vec{\theta}_0 = \vec{\theta}_1 = \vec{0}$, $\vec{\theta}_2 \neq \vec{0}$ (see Fig. 1 for definition of $\vec{\theta}_{0,1,2}$). The twisting angles are tuned to produce $q^2 = 0$ using two-point correlators fits according to

$$\vec{\theta}_1(q^2 = 0) = \frac{L}{\pi} \sqrt{\left(\frac{m_K^2 + m_\pi^2}{2m_\pi}\right)^2 - m_K^2}, \quad \vec{\theta}_2(q^2 = 0) = \frac{L}{\pi} \sqrt{\left(\frac{m_K^2 + m_\pi^2}{2m_K}\right)^2 - m_\pi^2}. \quad (2.3)$$

We found in a previous test run [7] that the use of random-wall sources greatly reduces the statistical errors of the parameters of the two-point and three-point correlators, so we use them throughout this analysis.

3. Simulation details and fitting

We have completed the generation of correlators with HISQ staggered valence quarks on the $2+1$ flavor asqtad staggered MILC ensembles [8] shown in Table 1 at two lattice spacings. We average results over four time sources separated by 16 (24) timeslices on the 0.12 fm (0.09 fm) ensembles but displaced by a random distance from configuration to configuration to suppress autocorrelations. A subset of this data was analyzed in [7]. The strange valence mass is tuned to its physical value on each ensemble [4]. The valence light-quark masses are fixed according to the relation, $\frac{m_l^{val}(HISQ)}{m_s^{phys.}(HISQ)} = \frac{m_l^{sea}(asqtad)}{m_s^{phys.}(asqtad)}$. The effect of the mixed actions for the sea and valence quark sectors can be analyzed using partially quenched staggered CHPT techniques for the chiral and continuum extrapolations.

	$\approx a$ (fm)	am_l/am_h	N_{conf}	am_s^{val}	am_l^{val}	$N_{sources}$	N_T
coarse	0.12	0.020/0.050	2052	0.0491(9)	0.02806	4	5
		0.010/0.050	2243	0.0495(9)	0.01414	4	8
		0.005/0.050	2098	0.0489(9)	0.00670	8	5
fine	0.09	0.0124/0.031	1996	0.0337(6)	0.0080	4	5
		0.0062/0.031	1946	0.0336(6)	0.0160	4	5

Table 1: Ensembles and simulation details. am_h is the nominal strange-quark mass in the sea sector, $N_{sources}$ is the number of time sources, and N_T the number of sink-source separations for which we have generated data.

We fit the two-point functions for a pseudoscalar meson P to the expression

$$C_{2pt}^P(\vec{p}_P; t) = \sum_{m=0}^{N_{exp}} (-1)^{mt} (Z_m^P)^2 \left(e^{-E_P^m t} + e^{-E_P^m (L_t - t)} \right), \quad (3.1)$$

where L_t is the temporal size of the lattice. Oscillating terms with $(-1)^m$ do not appear for pions with zero momentum. From two-point function fits, we checked whether the continuum dispersion relation is satisfied. This is plotted in Fig. 2, which shows very small deviations from the continuum prediction ($\leq 0.15\%$), indicating small discretization effects.

The functional form for the three-point functions is

$$C_{3pt}^{K \rightarrow \pi}(\vec{p}_\pi, \vec{p}_K; t, T) = \sum_{m,n=0}^{N_{exp}^{3pt}} (-1)^{mt} (-1)^{n(T-t)} A^{mn} Z_m^\pi Z_n^K \left(e^{-E_\pi^m t - E_\pi^m (L_t - t)} \right) \left(e^{-E_K^n (T-t) - E_K^n (T - L_t + t)} \right), \quad (3.2)$$

where the factors Z_i^P are the amplitudes of the two-point functions in (3.1). The three-point parameter A^{00} in (3.2) is related to the desired form factor $f_0^{K\pi}(q^2)$ via $f_0^{K\pi}(q^2) = \frac{1}{2} A^{00}(q^2) \sqrt{2E_\pi E_K} (m_s - m_l) / (m_K^2 - m_\pi^2)$, where we have used (2.2) and taken into account some overall factors involved in the parametrization of the correlation function. We extract the form factors $f_0^{K\pi}(q^2)$ using the expression above directly from simultaneous fits of the relevant three- and two-point functions. In these fits we include several three-point functions with different values of the source-sink separation T , with at least one odd T and one even T to be able to get a handle on the contributions from the oscillatory states.

In this analysis it is especially relevant to check for the stability of our fits under the choice of fitting parameters and techniques, since we are getting very small statistical errors and we need to be sure that these results are not methodology dependent in any way. One of the checks we performed is varying the time fitting ranges and number of states included in the fits. Fitting ranges for two-point functions are $t_{min} - (L_t - t_{min})$ and for the three-point functions $t_{min} - (T - t_{min})$, with L_t the temporal size of the lattice and T the source-sink separation—see Fig. 1. The number of states included is the same in the regular and oscillating sectors, so $N_{exp} = N_{regular\ states} = N_{oscillatory\ states}$. Fixing N_{exp} and changing t_{min} from 3 (5) for 0.12 fm (0.09 fm) ensembles up to the maximum allowed by the source-sink separation, give us a plateau for central values with only small variations in errors. Analogously, fixing t_{min} to our preferred value we do not find any significant variation of results for $N_{exp} \geq 3 - 4$.

We study as well which combination of T 's from the ones we have simulated is optimal. We find that the central values are very insensitive to the number of three-point functions included and the values of T in the range we are analyzing. Errors and stability are better when $15 \leq T \leq 24$ and including three three-point functions for the 0.12 fm ensembles, and $18 \leq T \leq 33$ and including four three-point functions for the 0.09 fm ensembles.

Finally, we checked an alternative way of doing the fits, using the iterative superaverage method described in [9]. This takes an explicit combination of three-point functions with consecutive values of T and the time slice t which suppresses the contribution from both the first regular excited state and the first oscillatory state. Again, results are compatible within one statistical σ with our preferred fitting method.

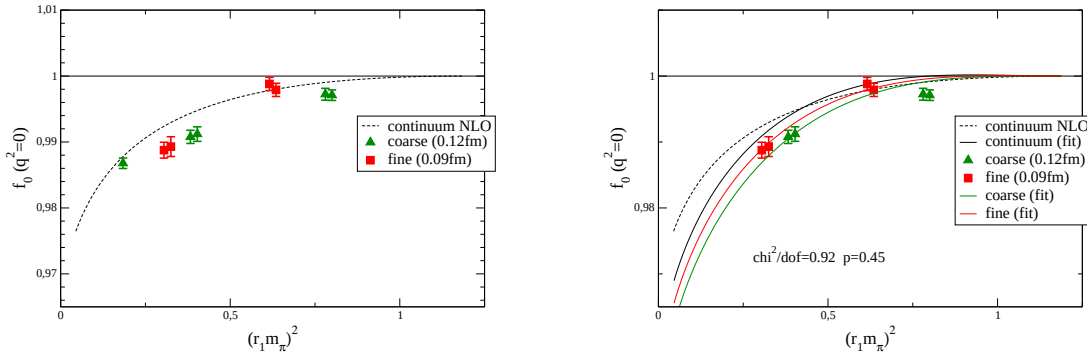


Figure 3: In the left panel, we collect the form factor $f_+^{K\pi}(0)$ obtained from the different ensembles in Table [1]. The right panel shows an example of the output from the chiral and continuum extrapolation tests. The dotted black line in both plots is the NLO CHPT prediction. The solid black line is the extrapolation in the light-quark mass with a physical m_s and in the continuum limit. The green and red lines are also extrapolations in the light-quark masses with m_s^{phys} but with $a \approx 0.12$ fm, 0.09 fm, respectively.

4. Results for $f_+(q^2 = 0)$

In Fig. 3 we collect the results for $f_+^{K\pi}(0)$ with statistical errors from our preferred fits as a function of $(r_1 m_\pi)^2$, fixing $(2m_K^2 - m_\pi^2)$ to the experimental value. We plot results coming from three-point functions where the external momentum to obtain $q^2 = 0$ is injected via the K and the π (we give an offset in the pion mass to the two points for clarity). The green triangle at the far left corresponds to the 0.12 fm ensemble with masses 0.005/0.050, four time sources, and a moving pion. When analyzing those data we found it to be more challenging to get stable results, so we have decided to double the number of sources and exclude it in our discussions until the full new data set is analyzed and other effects, like finite volume corrections, are incorporated to the analysis. So, in particular, we do not include it in the fits described below.

The first remarkable characteristic of our results is that the statistical errors are very small, 0.1 – 0.15%, reaching our goal to be competitive with other determinations. In addition, the results coming from three-point functions where the external momentum to get $q^2 = 0$ is injected via the K and the π agree within the very small statistical errors, as can be seen in the figure. This constitutes a very good test of our methodology and quoted errors.

4.1 Chiral and continuum extrapolation

The form factor $f_+(0)$ can be written as a CHPT expansion in the following way: $f_+(0) = 1 + f_2 + f_4 + f_6 + \dots = 1 + f_2 + \Delta f$. The Ademollo-Gatto (AG) theorem, which follows from vector current conservation, ensures that $f_+(0) \rightarrow 1$ in the $SU(3)$ limit and, furthermore, that the $SU(3)$ breaking effects are second order in $(m_K^2 - m_\pi^2)$. This fixes f_2 completely in terms of experimental quantities. At finite lattice spacing, systematic errors can enter due to, for example, corrections to the dispersion relation needed to derive Eq. (2.2). Those and other discretization effects are very small though, as can be deduced from our results in Fig. 3. However, since statistical errors are at the 0.1 – 0.2% level, we should pin down the other sources of systematic errors as precisely as possible.

Our plan for treating the light-quark mass dependence and the discretization effects in our calculation is to use two-loop continuum CHPT [10], supplemented by staggered partially quenched CHPT at one-loop. The small variation with a in our data suggests that addressing those effects at one loop should be enough for our target precision.

Since we do not yet have the staggered CHPT expressions, nor have we implemented the two-loop continuum CHPT functions, just as an exercise, we can try to fit our data with a much more simple fitting ansatz. We take the continuum partially quenched NLO CHPT expression [11] and add a general parametrization of NNLO analytic terms and a^2 corrections of the form

$$f_+^{K\pi}(0) = 1 + f_2 + C_a \left(\frac{a}{r_1} \right)^2 + r_1^4 (m_\pi^2 - m_K^2)^2 \left[C_6^{(1)} (r_1 m_\pi)^2 + C_6^{(2)} (r_1 m_K)^2 + C_6^{(3)} (r_1 m_\pi)^2 \log(m_\pi^2 / \mu^2) + C_6^{(4)} (r_1 m_\pi)^4 + C_6^{(5)} \left(\frac{a}{r_1} \right)^2 \right]. \quad (4.1)$$

We include only correlation functions coming from injecting the momentum in the π for these test fits. The result for one of these fits with $C_a = C_6^{(i)} = 0$ for $i = 3, 4$ is shown in Fig. 3. We can obtain similar good fits with different combinations of terms in (4.1). This must be taken just as a naive first try to fit our data and no conclusions should be drawn until we have used staggered CHPT to gain more information about the a^2 structure of our data.

5. Conclusions and outlook

We have completed the generation of the data in Table 1 needed for the calculation of $f_+^{K\pi}(0)$. Since the time of the conference we have generated data for another coarse ensemble with light-quark mass $am_l = 0.007$ to facilitate the chiral extrapolation, which we anticipate is going to be our main source of uncertainty.

The statistical errors in the form factor in all ensembles exceed our expectations, being around 0.1 – 0.15%. We have performed several checks of the robustness of the central fit values and errors, by studying the stability with changes in the time range and number of states, the dependence on the source-sink separation and number of three-point functions included in the fit, and testing alternative methods for fitting the correlation functions. We find it very difficult to make changes in the fitting procedure that change the fit results outside the one sigma range. Another very good test of our results is the fact that $f_+^{K\pi}(0)$ as extracted from three-point correlation functions with

a moving π and a moving K agree with each other. For the final analysis we will redo the fits we found to be the optimal, including the correlation functions with both momentum injected in the π and the K to further increase the statistics.

We found very small lattice spacing dependence in our data and the continuum dispersion relation is fulfilled at the 0.15% level, but in view of the small statistical error, we plan to study in detail the dependence on a^2 by using staggered partially quenched CHPT at one-loop. We will also investigate the use of two-loop continuum CHPT.

With all these elements, we expect our calculation to be competitive with the current state of the art.

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References

- [1] M. Antonelli *et al.*, Eur. Phys. J. **C69**, 399-424 (2010). [arXiv:1005.2323 [hep-ph]].
- [2] H. Na, C. T. H. Davies, E. Follana, G. P. Lepage, J. Shigemitsu, Phys. Rev. **D82** (2010) 114506. [arXiv:1008.4562 [hep-lat]].
- [3] V. Lubicz *et al.* [ETM Collaboration], Phys. Rev. **D80** (2009) 111502. [arXiv:0906.4728 [hep-lat]]; P. A. Boyle *et al.*, Eur. Phys. J. **C69** (2010) 159-167. [arXiv:1004.0886 [hep-lat]].
- [4] C. T. H. Davies, E. Follana, I. D. Kendall, G. P. Lepage and C. McNeile [HPQCD Collaboration], Phys. Rev. D **81** (2010) 034506 [arXiv:0910.1229 [hep-lat]].
- [5] P. F. Bedaque, J. -W. Chen, Phys. Lett. **B616**, 208-214 (2005). [hep-lat/0412023].
- [6] P. A. Boyle *et al.* [RBC-UKQCD Collaboration], Eur. Phys. J. **C69** (2010) 159-167. [arXiv:1004.0886 [hep-lat]].
- [7] J. A. Bailey *et al.* [Fermilab Lattice and MILC Collaboration], PoS **LATTICE2010** (2010) 306. [arXiv:1011.2423 [hep-lat]].
- [8] A. Bazavov *et al.*, Rev. Mod. Phys. **82** (2010) 1349-1417. [arXiv:0903.3598 [hep-lat]].
- [9] J. A. Bailey *et al.*, Phys. Rev. **D79** (2009) 054507. [arXiv:0811.3640 [hep-lat]].
- [10] J. Bijnens, P. Talavera, Nucl. Phys. **B669** (2003) 341-362. [hep-ph/0303103].
- [11] Johan Bijnens, private communication.

Properties of light pseudoscalars from lattice QCD with HISQ ensembles

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We fit lattice-QCD data for light-pseudoscalar masses and decay constants, from HISQ configurations generated by MILC, to SU(3) staggered chiral perturbation theory. At present such fits have rather high values of $\chi^2/\text{d.o.f.}$, possibly due to the lack of ensembles with lighter-than-physical sea strange-quark masses. We propose solutions to this problem for future work. We also perform simple linear interpolations near the physical point on two ensembles with different lattice spacings, and obtain the preliminary result $(f_K/f_\pi)^{\text{phys}} = 1.1872(41)$ in the continuum limit.

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1. Introduction

A great deal of interesting physics is accessible from the detailed study of the decay constants and masses of the light pseudoscalar mesons. For example, a determination of the decay constant ratio f_K/f_π provides a competitive determination of the CKM matrix element $|V_{us}|$, but the lattice errors limit the precision of the result [1]. Similar fits can give ratios of light-quark masses, and with nonperturbative or perturbative renormalization, absolute values of the masses themselves. In addition, chiral fits make possible the determination of important low-energy constants. Here we present a preliminary study of light pseudoscalar meson masses and decay constants using the highly improved staggered quark (HISQ) action [2]. The MILC collaboration has been generating HISQ configurations [3, 4], which are expected to improve upon results from the “asqtad” staggered quark action. We attempt to fit the light pseudoscalar data with SU(3) staggered chiral perturbation theory (ChPT). Since data exists for light- and strange-quark masses that are very nearly physical, we also perform simple linear interpolations of the data to the actual physical point and obtain a preliminary result for $(f_K/f_\pi)^{phys}$.

2. Ensembles and Correlators

Several ensembles have been generated by the MILC collaboration using the HISQ action, with 2+1+1 dynamical flavors and lattice spacings ranging from approximately 0.06 fm – 0.15 fm. The ensembles used in this report are found in Table 1. We use a notation in which m_l is the common mass of the up and down sea quark, m_s the mass of the strange sea quark, and m_c the mass of the charm sea quark. Note that two ensembles have nearly physical m_l , m_s , and m_c . Valence quarks are called x and y , and their masses are denoted by m_x and m_y respectively. Pseudoscalar mesons with valence quarks x and y have mass m_{xy} and decay constant f_{xy} .

Quark propagators were generated with various sources and sinks, with 8 – 10 different valence-quark masses depending on the particular ensemble, and in the approximate range $m_l^{phys} - m_s^{phys}$, where m_l^{phys} and m_s^{phys} are the physical light- and strange-quark mass. (Propagators with valence-quark mass $0.9m_c^{phys}$ and m_c^{phys} were also generated for heavy-light physics, but were not used in this report.) From these propagators, pseudoscalar meson correlators were calculated with random-wall and Coulomb-wall sources, and point sinks. The random-wall and Coulomb-wall correlators were fit simultaneously with independent amplitudes and a common mass. Only the amplitude from the random-wall correlators was used to obtain the decay constant. Four different time slices on each lattice were used for the source locations, with the locations of these slices shifting as we went through successive configurations.

The fits started at a time t_{min} from the source corresponding to ~ 2.4 fm in physical units for all of the lattice spacings. This choice was made by examining, on all of the ensembles, the dependence of fitted quantities on t_{min} . Fits including excited states and states of the opposite parity (“alternating states”) did not improve the quality of the fit, so they were not used. The exception was one of the ensembles with a nearly physical light-quark mass, which required adding an alternating state.

We attempt to account for autocorrelations in the covariance matrix of the fitted masses and decay constants by using the following *scaled* covariance matrix in our chiral fits:

$$D_{ij}^{[b]} \equiv C_{ij} \sqrt{r_i^{[b]} r_j^{[b]}}, \quad \text{where} \quad r_i^{[b]} = \frac{C_{ii}^{[b]}}{C_{ii}}. \quad (2.1)$$

a (fm)	am_l	am_s	am_c	N_{lats}
0.15	0.013	0.065	0.838	1020
0.15	0.0064	0.064	0.828	1000
0.12	0.0102	0.0509	0.635	1040
0.12	0.00507	0.0507	0.628	1020, 1000, 340*
0.12	0.00507	0.0304	0.628	1020
0.12	0.00184	0.0507	0.628	500**
0.09	0.0074	0.037	0.44	1011
0.09	0.00363	0.0363	0.43	633
0.09	0.0012	0.0363	0.432	248**
0.06	0.0048	0.024	0.286	503
0.06	0.0024	0.024	0.286	280

Table 1: HISQ ensembles used in this report. A single star indicates three different ensembles that have all the same parameters but different spatial volumes ($L/a = 24, 32, 40$). Two stars indicate ensembles where all quark masses are nearly physical. Note that all strange and charm quark masses are tuned to be nearly physical, except for the third ensemble with $a = 0.12$ fm, where the strange-quark mass is taken to be approximately 3/5 the physical value.

Here C_{ij} is an element of the original covariance matrix, and $C_{ij}^{[b]}$ is the corresponding element of the covariance matrix after blocking the configurations with block size b . Note that the scaled covariance matrix only uses the diagonal elements of the blocked covariance matrix $C_{ii}^{[b]}$. This is necessary because we use blocks of size $b = 10$, and not all of the off-diagonal elements of $C_{ij}^{[b]}$ can be determined with good accuracy.

3. Scale Setting

Before proceeding to do combined chiral fits of all the ensembles, it is necessary to determine accurately the *relative* scale between ensembles with different lattice spacings. For each lattice spacing we take the ensemble with $m_l = 0.1m_s$, and m_s near the physical strange-quark mass. We look at masses m_{xx} , and decay constants f_{xx} , *i.e.*, for pseudoscalars with two valence quarks of equal mass m_x . Looking at the dimensionless ratio f_{xx}/m_{xx} as a function of m_x , we find the value of m_x for which $f_{xx}/m_{xx} = R$, where R is some fiducial value. We take $R = 0.3575$, which is the value of f_{xx}/m_{xx} at $m_x = 0.4m_s^{phys}$, $m_l = 0.1m_s^{phys}$, and $m_s = m_s^{phys}$, as determined from a previous analysis using the asqtad action [5]. We give to this value of m_x the name “ m_{p4s} ”, or just m_p for short, and the values of f_{xx} and m_{xx} at this point are called “ f_{pp} ” and “ m_{pp} ”. Thus we expect to find that $m_p \approx 0.4m_s$ on each of the HISQ ensembles we are using to set the relative scale, and the extent to which this is not true depends on the accuracy of the tuning of m_s to the physical strange-quark mass, an issue to which we will return later. (We ignore any possible mistuning of the charm mass as a small effect).

In practice, we determine am_p by looking at the three sets of valence masses $am_x = 0.3am_s$, $0.4am_s$, and $0.6am_s$, and putting a parabola through m_{xx}^2/f_{xx}^2 vs. am_x . Once we have determined am_p and af_{pp} for a given lattice spacing, we can divide af_{xy} and am_{xy} by af_{pp} for that lattice spacing, and similarly we can divide quark masses am_x , am_y , am_l , etc., by am_p . This puts everything in “p4s

units”. Quantities in p4s units are dimensionless quantities that are comparable between ensembles with different lattice spacings.¹ With all quantities in p4s units, a combined chiral fit can be carried out. The advantage of our method is twofold. First, since the unphysical “p4s point” is well within the parameters of the data set, it can be reached by simple interpolation. Second, masses and decay constants at this point tend to have smaller errors than other quantities that could be used to set the scale. Our method is similar to the scaling trajectory method of [6].

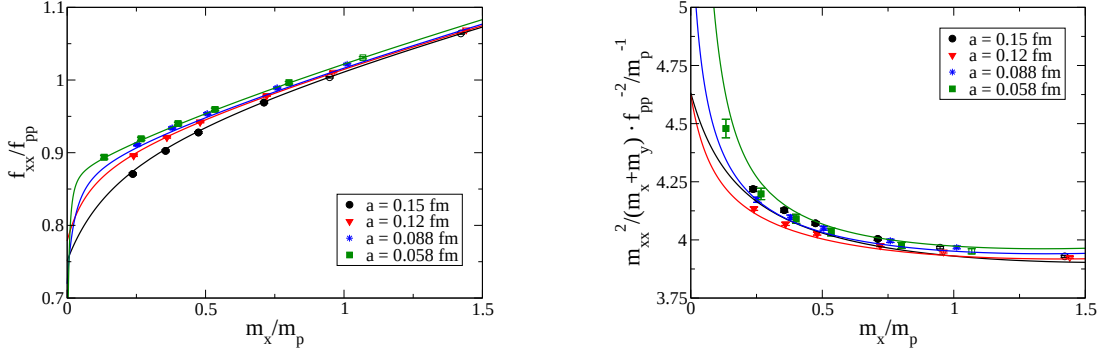
4. SU(3) Staggered Chiral Fits

We use SU(3), partially quenched, rooted, staggered ChPT to fit the pseudoscalar masses and decay constants as a function of valence- and sea-quark mass. The NLO expressions for the pseudoscalar mass and decay constant are given in Refs. [7] and [8], respectively. In our fits, we also include NNLO continuum terms from Ref. [9], and add even higher-order analytic terms, which is similar to the previous asqtad analysis of Ref. [5]. In order to obtain a reasonable fit to ChPT, we find it necessary to impose a cutoff on the valence quark masses: $m_x + m_y \leq 0.6(m_l + m_s)$. Also, our correlation matrix is close to singular, thus we smooth it by replacing all eigenvalues below 10^{-5} with their average. This is done as a quick fix in order to obtain preliminary results, and in future fits we will thin the data set instead.

We show the results of the fit on a subset of the data in Figure 1. The fit seems quite good to the eye, however when the covariances are included we see that the fit is not satisfactory: we get $\chi^2/\text{d.o.f.} = 1747/380 = 4.6$. If we do separate fits for each lattice spacing we get $\chi^2/\text{d.o.f.} = 1.9, 4.7, 2.6,$ and 0.7 for $a = 0.15$ fm, 0.12 fm, 0.09 fm, and 0.06 fm respectively. As discussed in Sec. 3, we assume that m_s is equal to the physical strange-quark mass when we set the relative scale, which can be checked by seeing if $m_p/m_s = 0.4$. In fact, we find $0.37 \lesssim m_p/m_s \lesssim 0.43$ for the different lattice spacings, indicating some mistuning of m_s . However, this cannot completely explain the poor fit because the $\chi^2/\text{d.o.f.}$ is still large for fits to ensembles at single lattice spacings, where no scale setting is necessary.

Another possible reason for the lack of a good fit is that quark masses are too large for SU(3) ChPT to work well, at least at the order to which we are working. In the asqtad analysis, this problem was dealt with by doing an initial fit with only lighter quark masses to fix LECs up to NNLO (and thereby controlling the extrapolation to m_l^{phys}), and then using the full set of quark masses to interpolate in the region of m_s^{phys} [5]. For the data set of this report (see Table 1), we only have one lighter-than-physical value of m_s , so we cannot do something similar, at least in the sea sector. New ensembles are being generated that will make this possible in future work. Another possibility is to use SU(2) ChPT, in which the strange quark is considered heavy, to fit the data. Staggered ChPT expressions for masses and decay constants have now been worked out for the SU(2) case [10].

¹That is, if we knew f_{pp} in MeV, then any meson mass or decay constant in p4s units from any lattice spacing would only need to be multiplied by this single number to put it in physical units. A similar comment applies for m_p and the quark masses.



(a) Pseudoscalar decay constant as a function of $m_x = m_y$.

(b) Pseudoscalar mass squared over the sum of the valence quark masses as a function of $m_x = m_y$.

Figure 1: Plots of the pseudoscalar mass and decay constant, and the fit to the data using SU(3) ChPT. We show only pions in these plots, *i.e.* $m_x = m_y$ which is shown on the x -axis. Data on the plots are for all of the different lattice spacings, (shown in different colors), but only for ensembles with $m_l = 0.2m_s$.

5. Linear Interpolations Near the Physical Point

In Table 1 we see that there are two ensembles with a nearly physical light sea-quark mass. Since we also have valence quarks with nearly physical light- and strange-quark masses, we can do a linear interpolation or extrapolation as necessary to the exact physical point. Figure 2 shows plots of m_{xy}^2 and f_{xy} vs. $m_x + m_y$ for one of the ensembles with nearly physical sea-quark masses. The plot of m_{xy}^2 is remarkably linear. The plot of f_{xy} is linear for small quark masses, but when one of the valence-quark masses m_y is heavier, the slope starts to depend on m_y . The situation is similar for the other ensemble, not shown.

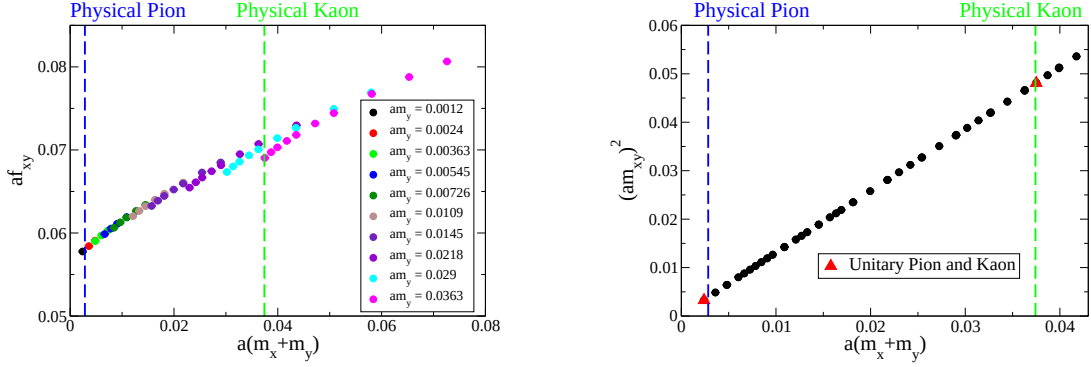
The observations of the previous paragraph suggest the following analytic fit form for a single ensemble:

$$(am_{xy})^2 = \begin{cases} (am_{\pi})^2(m_x, m_y) \equiv A_1 + B_1 a(m_x + m_y - 2m_l), & (m_x, m_y) \text{ near } (m_l, m_l), \\ (am_K)^2(m_x, m_y) \equiv A_2 + B_2 a(m_x + m_y - m_l - m_s), & (m_x, m_y) \text{ near } (m_l, m_s), \end{cases} \quad (5.1)$$

$$af_{xy} = \begin{cases} af_{\pi}(m_x, m_y) \equiv C_1 + D_1 a(m_x + m_y - 2m_l), & (m_x, m_y) \text{ near } (m_l, m_l), \\ af_K(m_x, m_y) \equiv C_2 + D_2 a(m_x - m_l) + E_2 a(m_y - m_s), & (m_x, m_y) \text{ near } (m_l, m_s). \end{cases} \quad (5.2)$$

We determine the values of the unknown coefficients $A_i - E_i$ using data for am_{xy} and af_{xy} at $(m_x, m_y) = (m_l, m_l)$, (m_l, m_s) , and the nearest neighboring points $(m_x, m_y) = (m_l, m^{(1)})$, $(m^{(1)}, m_s)$, and $(m_l, m^{(2)})$, where $m^{(1)}$ is near m_l and $m^{(2)}$ is near m_s . For the ensemble with $a = 0.09$ fm, we have $am_l = 0.0012$, $am_s = 0.0363$, $am^{(1)} = 0.0024$, and $am^{(2)} = 0.029$.

Keeping the sea-quark masses fixed by continuing to work within each ensemble, we then wish to determine am_l^{phys} and am_s^{phys} , where m_l^{phys} and m_s^{phys} are the quark masses that correspond to the physical point. Here we ignore the sea-quark masses entirely which introduces only a small



(a) Plot of f_{xy} vs. $m_x + m_y$. Points corresponding to different fixed values of am_y are indicated with different colors.

(b) Plot of m_{xy}^2 vs. $m_x + m_y$. The unitary points for this ensemble are indicated in red.

Figure 2: Plots of m_{xy}^2 and f_{xy} vs. $m_x + m_y$ for the ensemble with $a = 0.09$ fm, $am_l = 0.0012$, $am_s = 0.0363$, and $am_c = 0.432$. The values of $m_x + m_y$ corresponding to the physical pion and kaon mass are shown as blue and green dashed lines respectively. These were determined using Eq. 5.3.

partial quenching error because they are already close to physical. We set

$$\frac{af_\pi(m_l^{phys}, m_l^{phys})}{am_\pi(m_l^{phys}, m_l^{phys})} = \frac{f_\pi^{exp}}{m_\pi^{exp}}, \quad \frac{am_K(m_l^{phys}, m_s^{phys})}{am_\pi(m_l^{phys}, m_l^{phys})} = \frac{m_K^{exp}}{m_\pi^{exp}}, \quad (5.3)$$

where f_π^{exp} , m_π^{exp} , and m_K^{exp} are the experimental values. We can solve the left-hand equation for the unknown value am_l^{phys} , and then solve the right-hand equation to determine the unknown value am_s^{phys} . This allows us to calculate the dimensionless ratio

$$\left(\frac{f_K}{f_\pi}\right)^{phys} = \frac{af_K(m_l^{phys}, m_s^{phys})}{af_\pi(m_l^{phys}, m_l^{phys})}. \quad (5.4)$$

Results for $(f_K/f_\pi)^{phys}$ are shown in Table 2 for the two different ensembles with nearly physical sea-quark masses. We also show a continuum extrapolation of $(f_K/f_\pi)^{phys}$ by assuming that it is linear in a^2 for non-zero lattice spacing. To estimate the effect of partial quenching due to the fact that we kept sea-quark masses fixed during the analysis, we perform a similar analysis with unitary points only, from several of the ensembles with $a = 0.12$ fm.² We find $(f_K/f_\pi)^{phys} = 1.1963(25)$, in agreement with the value of 1.1950(23) for the $a = 0.12$ fm ensemble from Table 2. This gives us confidence that partial quenching is a small effect compared to the statistical uncertainty.

6. Conclusion

We performed fits using SU(3) staggered ChPT to pseudoscalar masses and decay constants on HISQ lattices with several different lattice spacings. We were unable to obtain a satisfactory

²The reason this is not done in the first place is that it is only possible for $a = 0.12$ fm with the current ensembles, (there is no lighter-than-physical strange-quark mass for the other lattice spacings), and because the interpolations are between points that are significantly further apart.

a (fm)	am_l	$a\Delta m_l$	am_s	$a\Delta m_s$	$(f_K/f_\pi)^{phys}$
0.12	0.00184	0.00019	0.0507	0.0013	1.1950(23)
0.09	0.00120	0.00022	0.0363	-0.0003	1.1913(16)
Continuum extrap.					1.1872(41)

Table 2: Results of interpolations to the physical point for f_K/f_π . We perform a continuum extrapolation assuming that this quantity is linear in a^2 for non-zero lattice spacing. We also show the distance of the interpolation points from the base data point, i.e. $\Delta m_l = m_l^{phys} - m_l$ and $\Delta m_s = m_s^{phys} - m_s$.

fit, which could be due in part to strange-quark mistuning, and also possibly to the sea and valence strange-quark masses being too large for ChPT to work well. New ensembles with lighter sea strange-quark masses will allow us to address these issues in future work by 1) allowing us to correct for strange-quark mistuning, and 2) allowing us to use only lighter sea- and valence-quark masses to fix LECs to NNLO, and then to add higher order terms to interpolate near the strange mass using the heavier masses, which is an approach similar to Ref. [5]. We will also try using SU(2) staggered ChPT, which treats the strange quark as heavy. We were able to obtain the preliminary result $(f_K/f_\pi)^{phys} = 1.1872(41)$ using simple linear interpolations around data points with nearly physical quark masses. The error on our result is comparable to that on the average of lattice results: $(f_K/f_\pi)^{phys} = 1.193(5)$ [11, 12], however we have included only the statistical error in our result. When the full fit to a much larger set of data points is performed, we expect to be able to obtain a rather precise result.

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References

- [1] Nakamura, K. et al., J. Phys. G **37** (2010) 075021, and 2011 partial update for the 2012 edition.
- [2] Follana, E. et al., Phys. Rev. D **75** (2007) 054502, [hep-lat/0610092].
- [3] Bazavov, A. et al., Phys. Rev. D **82** (2010) 074501, [arXiv:1004.0342].
- [4] Bazavov, A. et al., PoS(Lattice 2010) 320 (2010), [arXiv:1012.1265].
- [5] Bazavov, A. et al., PoS(Lattice 2010) 074 (2010), [arXiv:1012.0868].
- [6] Aoki, Y. et al., Phys. Rev. D **84** (2011) 014503, [arXiv:1012.4178].
- [7] Aubin, C. and Bernard, C., Phys. Rev. D **68** (2003) 034014, [hep-lat/0304014].
- [8] Aubin, C. and Bernard, C., Phys. Rev. D **68** (2003) 074011, [hep-lat/0306026].
- [9] Bijmans, J. et al., Phys. Rev. D **73** (2006) 074509, [hep-lat/0602003].
- [10] Bernard, C., Du, X., and Lightman, M., manuscript in preparation.
- [11] Colangelo, G. et al., Phys. Rev. C **71** (2011) 1695, [arXiv:1011.4408].
- [12] Laiho, J., Lunghi, E., and Van de Water, R. S., Phys. Rev. D **81** (2010) 034503, updates in PoS (FPCP2010) 040 (2010) and at www.latticeaverages.org, [arXiv:0910.2928].

***B*- and *D*-meson decay constants from three-flavor lattice QCD**

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Abstract

We calculate the leptonic decay constants of $B_{(s)}$ and $D_{(s)}$ mesons in lattice QCD using staggered light quarks and Fermilab bottom and charm quarks. We compute the heavy-light meson correlation functions on the MILC asqtad-improved staggered gauge configurations which include the effects of three light dynamical sea quarks. We simulate with several values of the light valence- and sea-quark masses (down to $\sim m_s/10$) and at three lattice spacings ($a \approx 0.15, 0.12$, and 0.09 fm) and extrapolate to the physical up and down quark masses and the continuum using expressions derived in heavy-light meson staggered chiral perturbation theory. We renormalize the heavy-light axial current using a mostly nonperturbative method such that only a small correction to unity must be computed in lattice perturbation theory and higher-order terms are expected to be small. We obtain $f_{B^+} = 196.9(8.9)$ MeV, $f_{B_s} = 242.0(9.5)$ MeV, $f_{D^+} = 218.9(11.3)$ MeV, $f_{D_s} = 260.1(10.8)$ MeV, and the SU(3) flavor-breaking ratios $f_{B_s}/f_B = 1.229(26)$ and $f_{D_s}/f_D = 1.188(25)$, where the numbers in parentheses are the total statistical and systematic uncertainties added in quadrature.

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I. INTRODUCTION

Leptonic decays of B and D mesons, in which the hadron annihilates weakly to a W boson, are important probes of heavy-to-light quark flavor-changing interactions. When combined with a nonperturbative lattice QCD calculation of the heavy-light pseudoscalar meson decay constant, f_B or f_D , a precise experimental measurement of the leptonic decay width allows the determination of the Cabibbo-Kobayashi-Maskawa (CKM) quark-mixing matrix element $|V_{ub}|$ or $|V_{cd}|$. Conversely, if the relevant CKM matrix element is known from an independent process such as semileptonic decay or from CKM-unitarity constraints, a comparison of the decay constant from lattice QCD simulations with that measured by experiment provides a straightforward test of the Standard Model. As the lattice and experimental determinations become more precise, this test will become more sensitive and may ultimately reveal, through the appearance of a discrepancy, the presence of new physics in the quark flavor sector.

Improved determinations of the B meson decay constant f_B are of particular importance given the current, approximately $3\text{-}\sigma$ tension in the CKM unitarity triangle that may indicate the presence of new physics in B_d -mixing or $B \rightarrow \tau\nu$ decay [1–3]. The experimental uncertainty in the branching fraction $\mathcal{B}(B \rightarrow \tau\nu)$ is at present $\sim 30\%$ [4, 5], but this error is expected to be reduced to $\sim 10\%$ by Belle II at KEK- B in as little as five or six years [6, 7], at which point even modest improvements in the determination of f_B will significantly help constrain the apex of the CKM unitarity triangle and isolate the source of new physics [8].

Because leptonic decays are “gold-plated” processes in numerical lattice QCD simulations (they have a single stable hadron in the initial state and no hadrons in the final state [9]), they can be determined accurately using present lattice methods. Currently all realistic lattice calculations of $f_{D(s)}$ and $f_{B(s)}$ that include the effects of three light dynamical quarks use staggered lattice fermions [10, 11] for the up, down, and strange quarks. Because staggered fermions are computationally cheaper than other lattice fermion formulations, they allow for QCD simulations with dynamical quarks as light as $0.05m_s$, several lattice spacings, down to $a \approx 0.045$ fm, large physical volumes, and high statistics. This enables lattice determinations of many light-light and heavy-light meson quantities with controlled systematic uncertainties. The results of staggered lattice calculations are largely in excellent numerical agreement with experimental results [9]. This includes both postdictions, such as the pion and kaon decay constants [12], and predictions, as in the case of the B_c meson mass [13]. Such successes give confidence that further calculations using the same methods are reliable. This is essential if lattice QCD calculations of hadronic weak matrix elements are to be used to test the Standard Model and search for new physics.

The staggered dynamical quark simulations used here employ the fourth-root procedure (“rooting”) for eliminating unwanted extra quark degrees of freedom that arise from lattice fermion doubling. The rooting method is not standard quantum field theory, and at nonzero lattice spacing it leads to violations of unitarity [14–17] that can be considered nonlocal [18]. Nevertheless, there are strong arguments [19, 20] that the desired local, unitary theory of QCD is reproduced by the rooted staggered lattice theory in the continuum limit. Further, one can show [15, 21] that the unitarity-violating lattice artifacts in the pseudo-Goldstone boson sector can be described, and hence removed, using rooted staggered chiral perturbation theory (rSXPT), which is a low-energy effective description of the rooted staggered lattice theory [22–24]. When coupled with other analytical and numerical evidence (see Refs. [25–28] for reviews and Ref. [29] for a recent study), this gives us confidence that the rooting procedure is valid. Indeed, the validity of the rooted staggered lattice simulations is of critical

importance to flavor physics phenomenology, since a majority of the unquenched, three-flavor lattice results for hadronic weak matrix elements used to determine CKM matrix elements and as inputs to constraints on the CKM unitarity triangle come from such simulations [30].

In this paper, we present new results for the leptonic decay constants of heavy-light mesons containing bottom and charm quarks. We use the “2+1” flavor asqtad-improved gauge configurations made publicly-available by the MILC Collaboration [31]. These ensembles include the effects of three light, dynamical sea-quark flavors: one with mass m_h near m_s (the physical strange-quark mass) and the other two with mass m_l as small as $0.1m_h$. We generate light valence quarks for the B and D mesons using the same staggered action as in the sea sector, and generate heavy bottom and charm quarks using the clover action [32] with the Fermilab interpretation [33]. Because the Fermilab method uses knowledge of the heavy-quark limit of QCD to systematically eliminate heavy-quark discretization errors, exploiting ideas of Symanzik [34, 35] and of heavy-quark effective theory (HQET) [36–38], it is well-suited for both bottom and charm quarks. We simulate with many values for the light up/down quark mass (the mass of our lightest pion in both the sea and valence sectors is ≈ 250 MeV), and at three lattice spacings ranging from $a \approx 0.09$ fm to $a \approx 0.15$ fm. We then extrapolate our numerical lattice data to the physical up and down quark masses and continuum guided by expressions derived in staggered chiral perturbation theory for heavy-light mesons (HMS χ PT) [39–41].

We renormalize the heavy-light axial current with a mostly nonperturbative approach, computing the flavor-diagonal (heavy-heavy and light-light) renormalization factors nonperturbatively and then calculate the remaining flavor off-diagonal correction factor ($\rho_{A_{Qq}^4}$) in lattice perturbation theory [37, 42, 43]. This procedure has the advantage that $\rho_{A_{Qq}^4}$ is close to unity. Furthermore, tadpole diagrams cancel in the ratio needed to obtain $\rho_{A_{Qq}^4}$, thereby improving the convergence of the perturbative series. Empirically, the size of the 1-loop contribution to $\rho_{A_{Qq}^4}$ is found to be small.

Our results for the charmed-meson decay constants improve upon our published results for f_D and f_{D_s} in Ref. [44] in several ways. The coarsest lattices used in this work have a smaller lattice spacing ($a \approx 0.15$ fm) than those used in our previous work ($a \approx 0.18$ fm). The number of configurations in the two most chiral ensembles with $a \approx 0.12$ fm has been increased, approximately by factors of 1.4 (sea $m_l = 0.1m_h$) and 1.7 (sea $m_l = 0.14m_h$). We have added new data on a new $a \approx 0.09$ fm sea-quark ensemble with a light quark mass of $0.1m_h$. We now obtain our results from a combined analysis of our entire data set (all partially-quenched mass combinations and lattice spacings). Furthermore, we now compute the bottom meson decay constants f_B and f_{B_s} . We have presented reports on this project at several conferences [45–49]; in our final analysis of this data set we also improve upon bottom and charm quark mass-tuning, with increased statistics and a more sophisticated analysis of heavy-quark discretization effects.

This paper is organized as follows. In Sec. II, we present an overview of the calculation, including the gluon and light-quark actions used in generating the gauge configurations and the light- and heavy-quark actions used in constructing the heavy-light meson correlators. We also introduce the mostly nonperturbative method for matching the lattice heavy-light current to the continuum, and the treatment of heavy-quark discretization errors from the Fermilab action within our chiral-continuum extrapolation. Next, in Sec. III, we describe the details of our numerical simulations and we present the parameters used, such as the light-quark masses and lattice spacings. We also describe the procedure for tuning the hopping

TABLE I. Flavor content of the axial vector current and associated CKM matrix element.

H	$\mathcal{A}^\mu$	V
D	$\bar{d}\gamma^\mu\gamma^5 c$	V_{cd}^*
D_s	$\bar{s}\gamma^\mu\gamma^5 c$	V_{cs}^*
B	$\bar{b}\gamma^\mu\gamma^5 u$	V_{ub}
B_s	$\bar{b}\gamma^\mu\gamma^5 s$	—

parameter in the clover action so that it corresponds to b and c quarks. In Sec. IV, we define the two-point correlation functions used to extract the decay constant at each value of the light-quark mass and lattice spacing. We use two different fitting procedures to obtain the decay constants that differ in their treatment of the statistical errors, choice of fit ranges and number of states, and choice of input correlators. We include the difference between the two in our estimate of the fitting systematic uncertainty. Next, we present the numerical details of the calculation of the heavy-light axial-current renormalization factor in Section V. Putting the results of the two previous sections together, in Sec. VI, we extrapolate the renormalized decay constant data at unphysical quark masses and nonzero lattice spacing to the physical light quark masses and zero lattice spacing using HMS χ PT. In Sec. VII, we estimate the contributions of the various systematic uncertainties to the decay constants, discussing each item in our error budget separately. We present the final results for the decay constants in Sec. VIII, and compare them to other lattice QCD calculations and to experiment. We describe the impact of our results for current flavor physics phenomenology and then conclude by discussing the ongoing improvements to our calculations, and their future impact on searches for new physics in the quark flavor sector.

Appendix A applies HQET to the Fermilab action to obtain explicit expressions for heavy-quark discretization effects. Appendix B contains the complete set of fit results for the heavy-light pseudoscalar meson mass and renormalized decay constant for all combinations of sea-quark mass, light valence-quark mass, and heavy-quark mass used in the chiral-continuum extrapolation. These results will be included as an EPAPS attachment upon publication.

II. METHODOLOGY

The decay rate for a charged pseudoscalar meson H (with flavor content Q and $\bar{q}$) to leptons is, in the Standard Model,

$$\Gamma(H \rightarrow \ell\nu) = \frac{M_H}{8\pi} f_H^2 |G_F V_{Qq}^* m_\ell|^2 \left(1 - \frac{m_\ell^2}{M_H^2}\right)^2, \quad (2.1)$$

where M_H is the mass of the meson H , G_F is the Fermi constant, and V_{Qq} is the pertinent element of the CKM matrix. The decay constant f_H parameterizes the pseudoscalar-to-vacuum matrix element of the axial vector current,

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle = i p^\mu f_H, \quad (2.2)$$

where p^μ is the 4-momentum of the pseudoscalar meson. The flavor contents of the associated vector current and CKM matrix element are given in Table I. Note that the neutral B_s decays to a charged lepton pair with an amplitude proportional to f_{B_s} ; hence the CKM

factor in the decay rate involves more than one CKM matrix element. Because this process is loop-suppressed in the Standard Model, it is potentially sensitive to new physics effects. These formulas hold for all pseudoscalar mesons; in the normalization convention used here, $f_\pi(|V_{ud}|/0.97425) = 130.41 \pm 0.20$ MeV [50].

In Eq. (2.2), the 1-particle state assumes the relativistic normalization convention. For mesons containing a heavy quark, however, it is more convenient to pull out factors of M_H to ensure a smooth $M_H \rightarrow \infty$ limit:

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle (M_H)^{-1/2} = i(p^\mu / M_H) \phi_H. \quad (2.3)$$

In lattice QCD, the normalization of states on the left-hand side falls out of correlation functions more naturally. Thus, most of our analysis, including error analysis, focuses on ϕ_H . We then obtain $f_H = \phi_H / \sqrt{M_H}$ using the experimentally measured value of the meson mass [51].

To compute the decay constants with lattice gauge theory, we must choose a discretization for the heavy quark, the light quark, and the gluons. As in previous work [44, 52–55], we choose the Fermilab method for heavy quarks [33] and staggered quarks with the asqtad action [56] for the light (valence) quark. The gauge action is Symanzik improved, with couplings chosen to remove order $\alpha_s a^2$ errors from gluon loops [57], but not those from quark loops [58] (which became available only after the gauge-field generation was well underway).

For heavy bottom and charm quarks, we use the Sheikholeslami-Wohlert (SW) clover action [32] with the Fermilab interpretation [33], which connects to the continuum limit as $am_Q \rightarrow 0$. This is an extension of the Wilson action [59], which retains the Wilson action’s smooth limit as $am_Q \rightarrow \infty$ and also remains well behaved for $m_Q a \approx 1$. Because this lattice action respects heavy-quark spin-flavor symmetry, one can apply HQET to organize the discretization effects. In essence, one uses HQET to develop the $1/m_Q$ expansion both for continuum QCD and for lattice gauge theory (LGT) [36–38]. Discretization effects are then captured order-by-order in the heavy-quark expansion by the difference of the short-distance coefficients in the descriptions of QCD and LGT. Thus, in principle, the lattice heavy-quark action can be improved to arbitrarily high orders in $1/m_Q$ by adjusting a sufficiently large number of parameters in the lattice action. (See Ref. [60] for details at dimension 6 and 7. In principle, the adjustment can be done nonperturbatively, such as in the scheme of Ref. [61].) In practice, we tune the hopping parameter κ and the clover coefficient c_{SW} of the SW action, to remove discretization effects through order $1/m_Q$ in the heavy-quark expansion.

The HQET analysis of cutoff effects could be applied to any lattice action with heavy-quark symmetry, such as the action of lattice NRQCD [62]. In the latter case, it is simply a different perspective on the usual approach to lattice NRQCD, which derives the heavy-quark Lagrangian formally, and then replaces derivatives with difference operators. A key feature of the Wilson, SW, Fermilab and OK [60] actions is their well-behaved continuum limit, which is especially important for charm. For $m_Q a < 1$, one can analyze the cutoff effects in a complementary way with the Symanzik effective action [34, 35]. This two-pronged attack shows that the difference of short-distance coefficients, mentioned above, vanishes as a suitable power of lattice spacing a . In this paper, we shall use our knowledge of this behavior to constrain heavy-quark discretization effects in several steps of our analysis. See Secs. III B, VI, and Appendix A for details.

The lattice and continuum currents are related by a matching factor Z_{A^μ} [37]:

$$Z_{A^\mu} A^\mu \doteq \mathcal{A}^\mu + \mathcal{O}(\alpha_s a \Lambda f_i(m_Q a)) + \mathcal{O}(a^2 \Lambda^2 f_j(m_Q a)), \quad (2.4)$$

where $\doteq$ denotes equality of matrix elements, and the functions $f_{i,j}$ that depend on $m_Q a$ stem from the difference in the HQET short-distance coefficients. In the Fermilab method, they remain of order 1 for all values of $m_Q a$ [33, 60], and they are given explicitly in Appendix A. In this work, we compute Z_{A^μ} mostly nonperturbatively [42] and partly in one-loop perturbation theory. As shown in the analysis of Ref. [37], many of the Feynman diagrams in the perturbative expansion of $Z_{A_{Qq}^4}$ are common or similar to those in the flavor-conserving renormalization factors $Z_{V_{Qq}^4}$ and $Z_{V_{qq}^4}$, which can be computed nonperturbatively. Therefore, we define $\rho_{A_{Qq}^4}$ by

$$Z_{A_{Qq}^4} = \rho_{A_{Qq}^4} \sqrt{Z_{V_{qq}^4} Z_{V_{Qq}^4}}, \quad (2.5)$$

evaluating only $\rho_{A_{Qq}^4}$ in lattice perturbation theory.

The flavor-conserving factors account for most of the value of the heavy-light renormalization factor $Z_{A_{Qq}^4}$. They are obtained by enforcing the normalization condition, at zero momentum transfer,

$$1 = Z_{V_{qq}^4} \langle H_q | V_{qq}^4 | H_q \rangle, \quad (2.6)$$

where H_q is a hadron containing a single quark of flavor q , and V_{qq}^μ is the lattice version of the degenerate vector current. This condition holds for all discretizations and quark masses and, hence, the heavy quark (*i.e.*, $Z_{V_{Qq}^4}$) as well. The remaining correction factor $\rho_{A_{Qq}^4}$ is close to unity due to the cancellation of most of the radiative corrections including tadpole graphs. Although such cancellations have only been explicitly shown at 1-loop in lattice perturbation theory [37, 43], we expect similar cancellations to persist at higher orders. Therefore, the perturbative truncation error in the heavy-light renormalization factor is subdominant.

III. LATTICE SIMULATION DETAILS

A. Parameters

Table II lists the subset of the ensembles of lattice gauge fields generated by the MILC Collaboration [28] used in this analysis. We now describe each entry in the table.

We analyze data at three lattice spacings: $a \approx 0.15$ fm, $a \approx 0.12$ fm, and $a \approx 0.09$ fm. The ensembles contain 2+1 flavors of sea quarks, using the asqtad-improved staggered action [56], and the square (fourth) root of the staggered determinant for the two degenerate light sea quarks (one strange sea quark). The sea contains one flavor with mass m_h close to the physical strange quark mass and two degenerate lighter flavors of mass m_l . The tadpole improvement factor u_0 is a parameter of the gauge and asqtad staggered (sea) quark action and is determined from the fourth root of the average plaquette. We calculate the two-point correlation functions on each ensemble from an average over four different time sources.

The relative lattice scale is determined by calculating r_1/a on each ensemble, where r_1 is related to the force between static quarks, $r_1^2 F(r_1) = 1.0$ [63, 64]. Table II lists r_1/a values for each of the ensembles that result from fitting the calculated r_1/a to a smooth function [65], as explained in Eqs. (115) and (116) of Ref. [28].

TABLE II. The MILC three-flavor lattices and valence asqtad quark masses used in this work. All of the valence masses were used in version II of the correlator fits (Sec IV C), while only the ones in bold print were used in version I (Sec IV B).

$\approx a$ [fm]	am_h	am_l	u_0	r_1/a	$n_{\text{conf}} \times n_{\text{src}}$	valence am_q
0.09	0.031	0.0031	0.8779	3.69	435×4	0.0031 , 0.0037, 0.0042, 0.0044 , 0.0052, 0.0062 , 0.0087 , 0.0124 , 0.0186 , 0.0272 , 0.031
		0.0062	0.8782	3.70	557×4	0.0031 , 0.0037, 0.0044 , 0.0052, 0.0062 , 0.0087 , 0.0124 , 0.0186 , 0.0272 , 0.031
		0.0124	0.8788	3.72	518×4	0.0031 , 0.0042 , 0.0062 , 0.0087 , 0.0124 , 0.0186 , 0.0272 , 0.031
0.12	0.05	0.005	0.8678	2.64	678×4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.007	0.8678	2.63	833×4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.01	0.8677	2.62	592×4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.02	0.8688	2.65	460×4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
		0.03	0.8696	2.66	549×4	0.005 , 0.006, 0.007 , 0.0084, 0.01 , 0.012, 0.014 , 0.017, 0.02 , 0.024, 0.03 , 0.0415
0.15	0.0484	0.0097	0.8604	2.13	631×4	0.0048 , 0.007 , 0.0097 , 0.013, 0.0194 , 0.0242, 0.029 , 0.0387, 0.0484
		0.0194	0.8609	2.13	631×4	0.0048 , 0.007 , 0.0097 , 0.013, 0.0194 , 0.0242, 0.029 , 0.0387, 0.0484
		0.029	0.8614	2.13	576×4	0.0048 , 0.007 , 0.0097 , 0.013, 0.0194 , 0.0242, 0.029 , 0.0387, 0.0484

In order to fix the absolute lattice scale, one must compute a physical quantity which can be compared directly to experiment. The combination of the PDG's value of f_π with MILC's 2009 determination of $r_1 f_\pi$ [66] yields $r_1 = 0.3117(6)({}_{-31}^{+12})$ fm. From an average of three methods for scale setting, including one based on Υ splittings, the HPQCD collaboration obtains $r_1 = 0.3133(23)(3)$ fm [67], consistent with MILC. Symmetrizing MILC's error range gives $r_1 = 0.3108(21)$ fm, and a straightforward average with the HPQCD result then yields $r_1 = 0.3120(16)$ fm. This average omits likely correlations, due to the use of MILC sea-quark configurations by both groups. Conservatively assuming a 100% correlation, we inflate the error to 0.0022 fm. Finally, for convenience, we also shift the central value slightly, back to the 2009 MILC central value. We thus take $r_1 = 0.3117(22)$ fm in this paper.

The complete list of light (asqtad) valence quark masses m_q simulated in this analysis is also given in Table II. The mass values are selected to be roughly logarithmically spaced, but to also include the set of light sea quark masses simulated at each lattice spacing. We use a multimass solver to compute the valence quark propagators. The marginal numerical cost of including masses heavier than our lightest $m_q \sim 0.1m_s$ is small and logarithmic spacing is designed to constrain the chiral logarithms.

TABLE III. Table of clover coefficients and κ values for charm and bottom used in heavy-light two-point simulations.

$\approx a$ [fm]	am_l/am_h	c_{SW}	κ_{sim}	
			charm	bottom
0.09	0.0031/0.031	1.478	0.127	0.0923
	0.0062/0.031	1.476		
	0.0124/0.031	1.473		
0.12	0.005/0.05	1.72	0.122	0.086
	0.007/0.05	1.72		
	0.01/0.05	1.72		
	0.02/0.05	1.72		
	0.03/0.05	1.72		
0.15	0.0097/0.0484	1.570	0.122	0.076
	0.0194/0.0484	1.567		
	0.0290/0.0484	1.565		

In Table III, we show the coefficient of the Sheikholeslami-Wohlert term c_{SW} of the clover action and the κ values used to compute heavy-light two-point functions. The coefficient of the clover term is set to the tadpole-improved tree-level value $c_{\text{SW}} = u_0^{-3}$. For the $a \approx 0.09$ and 0.15 ensembles the tadpole coefficient is taken from the average plaquette. We note, however, that at lattice spacing $a \approx 0.12$ fm the tadpole coefficient u_0 appearing in both the valence asqtad action and the heavy quark clover action is taken from the average of the Landau link evaluated on the $am_l/am_h = 0.01/0.05$ ensemble. Hence, in our $a \approx 0.12$ fm lattice data there is a mismatch between light valence and sea quark mass definitions. As discussed in Sec. VII, this (inadvertent) choice leads to a small error in the decay constants. We have remedied this mismatch by using the plaquette u_0 everywhere in new runs started while this analysis was underway.

The charm and bottom kappa values listed in Table III are based on our initial kappa tuning analysis using about one fourth of our final statistics. We then used a larger data set to refine our determination of the κ values corresponding to bottom and charm as described in the next subsection. We adjust our data post-facto to correspond to tuned values of κ_c and κ_b using the measured value of the derivative $\delta\phi/\delta\kappa$.

B. Input quark masses m_c and m_b

Our method for tuning κ for charm and bottom quarks closely follows that of Ref. [55], where further details can be found. We start with the dispersion relation for a heavy particle on the lattice [33]

$$E^2(\mathbf{p}) = M_1^2 + \frac{M_1}{M_2} \mathbf{p}^2 + \frac{1}{4} A_4 (a\mathbf{p}^2)^2 + \frac{1}{3} A_4' a^2 \sum_{j=1}^3 |p_j|^4 + \dots, \quad (3.1)$$

where

$$M_1 \equiv E(\mathbf{0}) \quad (3.2)$$

TABLE IV. Hopping-parameter values used to compute the dispersion relation.

$\approx a$ [fm]	$n_{\text{conf}} \times n_{\text{src}}$	κ_Q	
		charm	bottom
0.09	1912×4	0.1240, 0.1255, 0.1270	0.090, 0.092, 0.094
0.12	592×4	0.114, 0.117, 0.119, 0.122, 0.124	0.074, 0.086, 0.093, 0.106
0.15	631×8	0.100, 0.115, 0.122, 0.125	0.070, 0.076, 0.080, 0.090

is called the rest mass, and the kinetic mass is given by

$$M_2^{-1} \equiv \left. \frac{\partial E(\mathbf{p})}{\partial p_j^2} \right|_{\mathbf{p}=\mathbf{0}}. \quad (3.3)$$

These meson masses differ from corresponding quark masses, m_1 and m_2 , by binding-energy effects. The bare mass or, equivalently, the hopping parameter κ must be adjusted so that these masses reproduce an experimental charmed or b -flavored meson mass. When they differ, as they do when $m_Q a \ll 1$, one must choose. Decay constants are unaffected by the heavy-quark rest mass m_1 [36], so it does not make sense to adjust the bare mass to M_1 . We therefore focus on M_2 , adjusting κ to the strange pseudoscalars D_s and B_s , both because the signal degrades for lighter spectator masses and because this avoids introducing an unnecessary systematic uncertainty due to a chiral extrapolation.

The first step is to compute the correlator $C_2^{(S_1 S_2)}(t, \mathbf{p})$ in Eq. (4.8) (below) for several 3-momenta $\mathbf{p}$ and several values of κ and light quark mass, bracketing charm and bottom, and strange, respectively. We use all momenta such that $|\mathbf{p}| \leq 4\pi/L$. Second, we fit the time dependence of the multichannel correlation matrix $C_2^{(S_1 S_2)}$ to a sum of exponentials—including the usual staggered-fermion oscillating terms—and extract the ground state energy $aE(\mathbf{p})$ by minimization of an augmented χ^2 [55, 68, 69]. Third, we fit the energies to the dispersion relation given in Eq. (3.1), through $\mathcal{O}(p_i^4)$. The output of this fit is aM_1 , M_1/M_2 , A_4 , and $A_{4'}$, all as functions of κ . Fourth, we form $M_2(\kappa)$ from the first two fit outputs and r_1/a , propagating the error with a single-elimination jackknife. Finally, we obtain our tuned κ_c and κ_b by interpolating in κ so that $M_2(\kappa)$ matches the experimentally known D_s and B_s masses. The κ values used to compute M_2 are listed in Table IV. For each of the lattice spacings listed, we used the ensemble with light-to-strange sea-quark mass ratio $am_l/am_h = 0.2$. The resulting tuned values of κ_c and κ_b are shown with errors in Table V.

We constrain the coefficients A_4 and $A_{4'}$ with Gaussian priors derived from the HQET theory of cutoff effects, adding the contribution of the priors to the χ^2 in the minimization procedure [68, 69]. (In principle, we could include such priors for M_1 and M_1/M_2 too, but in practice we take priors so wide that these fit parameters are solely data-driven.) Neglecting binding energies, we have exact tree-level expressions for a_4 and $a_{4'}$, the quark analogs of A_4 and $A_{4'}$. The differences $A_4 - a_4^{[0]}$ and $A_{4'} - a_{4'}^{[0]}$ stem from both perturbative and nonperturbative effects. The asymptotics of the former can be estimated along the lines of Appendix A 3, and the latter can be deduced following the methods of Refs. [36, 70]. Briefly, we constrain $A_n(\kappa)$, $n \in \{4, 4'\}$, to a Gaussian with central value

$$a_n^{[0]}(m_0 a) + \alpha_s a_n^{[1]}(m_0 a) + \bar{\Lambda} a A'_n(m_0 a). \quad (3.4)$$

Here $a_n^{[0]}$ is the exact tree-level contribution, $a_n^{[1]}$ is an estimate of the one-loop contribution, and A'_n is an expression for the binding-energy contribution. The width of the Gaussian is

TABLE V. Hopping parameter values κ_c and κ_b corresponding to charm and bottom. The outputs of the tuning are labeled κ_{tuned} , where the first error is from statistics and the second is from r_1 , which enters through matching to the experimentally-measured D_s and B_s meson masses. The derivative $d\phi/d\kappa$ is used to correct the values of ϕ obtained with the simulated values κ_{sim} listed in Table III to the tuned values given below.

$\approx a$ [fm]	charm		bottom	
	κ_{tuned}	$d\phi/d\kappa$	κ_{tuned}	$d\phi/d\kappa$
0.09	0.12691(18)(13)	-21.66	0.0959(13)(3)	-7.41
0.12	0.12136(37)(19)	-18.23	0.0856(19)(3)	-6.82
0.15	0.12093(36)(24)	-15.40	0.0788(11)(3)	-6.07

determined by combining in quadrature the chosen widths of the separate contributions, as outlined in Appendix A 3.

The details of the κ_c and κ_b determination differ from that of Ref. [55] in two respects. First, we use the pseudoscalar meson masses rather than the spin average of pseudoscalar and vector meson masses, leading to a modest reduction of the statistical error. Second, we include the quartic terms in Eq. (3.1), allowing us to fold discretization effects directly into the dispersion-relation fit. Although we consider these two changes improvements, the change in the tuned κ values as compared to Ref. [55] stems primarily from the substantial increase in statistics on key ensembles.

The computations of the correlation functions needed to extract ϕ_D and ϕ_B have been carried out using the fiducial values listed in Table III. These simulation κ 's were obtained near the beginning of the project, but while the runs were in progress, we redetermined the hopping parameters utilizing increased statistics and reflecting an updated value of r_1 [66]. The resulting improved determinations of κ_c and κ_b differ slightly from the simulation values. In order to adjust ϕ from the simulated value κ_{sim} to the tuned value κ_{tuned} , we write

$$\phi_{\text{tuned}} = \phi_{\text{sim}} + \frac{d\phi}{d\kappa}(\kappa_{\text{tuned}} - \kappa_{\text{sim}}), \quad (3.5)$$

where the derivatives $d\phi/d\kappa$ listed in Table V are obtained from tuning runs with nearby κ values. As explained in Sec. VII, these derivatives are also used to propagate to the decay constants the statistical and scale uncertainties on κ_{tuned} listed in Table V.

IV. TWO-POINT CORRELATOR FITS

We obtain the unrenormalized decay amplitude for every combination of heavy-quark mass, light-quark mass, and sea-quark ensemble by fitting the heavy-light meson two-point correlation functions, described in Sec. IV A. We use two independent fitting procedures, which we refer to as “Analysis I” and “Analysis II”. These procedures differ in several respects. In Analysis I, we use a jackknife procedure for estimating errors, while in Analysis II, we use a bootstrap procedure. The two analyses also differ in their methods for handling autocorrelations in the data and in their choices of fit ranges, priors for masses and amplitudes, and numbers of states included. In the end, we use Analysis I (Sec. IV B) to obtain central values, and use differences from fits with different distance ranges and/or number

of states included, and from Analysis II (Sec. IV C) to estimate the systematic error due to choices made in the fit procedure.

A. Lattice correlators

The lattice axial-vector current is given by

$$A_a^4(x) = [\bar{\Psi}(x)\gamma^4\gamma^5\Omega(x)]_a\chi(x), \quad (4.1)$$

where $\chi(x)$ is the one-component field appearing in the staggered action, and $\Omega(x) = \gamma_1^{x_1/a}\gamma_2^{x_2/a}\gamma_3^{x_3/a}\gamma_4^{x_4/a}$ is the transformation connecting naive and staggered fields [71]. The heavy-quark field Ψ is a four-component (Dirac) spinor field, and the remaining free Dirac index is interpreted as a taste label.

To remove tree-level discretization errors in the lattice axial current, the heavy-quark field Ψ is “rotated”:

$$\Psi = [1 + ad_1\boldsymbol{\gamma} \cdot \mathbf{D}]\psi, \quad (4.2)$$

where ψ is the field appearing in the clover action. Tree-level improvement is obtained when

$$d_1 = \frac{1}{2 + m_0a} - \frac{1}{2(1 + m_0a)}, \quad (4.3)$$

where

$$m_0a = \frac{1}{u_0} \left(\frac{1}{2\kappa} - \frac{1}{2\kappa_{\text{crit}}} \right) \quad (4.4)$$

is the tadpole-improved bare mass. The critical hopping parameter κ_{crit} is the one for which the clover-clover pion mass vanishes.

As usual in lattice gauge theory, we obtain the matrix element in (2.3) from two-point correlation functions. We introduce pseudoscalar operators

$$\mathcal{O}_a^{(S)}(x) = \sum_y [\bar{\psi}(y)S(y, x)\gamma^5\Omega(x)]_a\chi(x), \quad (4.5)$$

depending on a “smearing” function S . In this work, we use two functions, the local (or unsmeared) source $S(x, y) = \delta_{xy}$, and the smeared source (in Coulomb gauge)

$$S(x, y) = \delta_{x_4y_4}S(\mathbf{x} - \mathbf{y}), \quad (4.6)$$

where $S(\mathbf{r})$ is the $1S$ solution of the Richardson potential for the quarkonium systems [72]. We obtain $S(\mathbf{x} - \mathbf{y})$ by scaling the radial Richardson wavefunction to lattice units, interpolating it to lattice sites, and then using it as the spatial source for the heavy-quark propagators [73].

We introduce two-point correlation functions

$$\Phi_2^{(S)}(t) = \sum_{a=1}^4 \sum_{\mathbf{x}} \left\langle A_a^{4\dagger}(t, \mathbf{x}) \mathcal{O}_a^{(S)}(0) \right\rangle, \quad (4.7)$$

$$C_2^{(S_1 S_2)}(t, \mathbf{p}) = \sum_{a=1}^4 \sum_{\mathbf{x}} e^{i\mathbf{p} \cdot \mathbf{x}} \left\langle \mathcal{O}_a^{(S_1)\dagger}(t, \mathbf{x}) \mathcal{O}_a^{(S_2)}(0) \right\rangle, \quad (4.8)$$

where $\langle \bullet \rangle$ now represents the ensemble average. For large time separations, $\Phi_2^{(S)}$ is proportional to the matrix element ϕ_H , and the proportionality is determined from $C_2^{(SS)}(t, \mathbf{0})$. Each two-point function is constructed from a staggered quark propagator with local (δ) sources and sinks. We compute C_2 functions for all (four) combinations $S_1, S_2 = \delta$ and $1S$, requiring heavy clover quark propagators with all combinations of $1S$ smeared and local sources and sinks. Only the local sink clover propagators are needed to compute the Φ_2 functions. With the sum over tastes in Eqs. (4.7) and (4.8), the correlation functions Φ_2 and C_2 can also be cast in a heavy-naive formalism [74].

The staggered light quarks in the axial-current and pseudoscalar two-point correlation functions lead to the presence of opposite-parity states that oscillate in time as $(-1)^t$. Hence the two-point functions take the following forms:

$$\begin{aligned} \Phi_2^{(S)}(t) = & A_{\Phi}^{(S)} (e^{-Mt} + e^{-M(T-t)}) + \tilde{A}_{\Phi}^{(S)} (-1)^t (e^{-\tilde{M}t} + e^{-\tilde{M}(T-t)}) \\ & + A_{\Phi}'^{(S)} (e^{-M't} + e^{-M'(T-t)}) + \dots, \end{aligned} \quad (4.9)$$

$$\begin{aligned} C_2^{(S_1 S_2)}(t, \vec{p} = 0) = & A^{(S_1)} A^{(S_2)} (e^{-Mt} + e^{-M(T-t)}) + \tilde{A}^{(S_1)} \tilde{A}^{(S_2)} (-1)^t (e^{-\tilde{M}t} + e^{-\tilde{M}(T-t)}) \\ & + A'^{(S_1)} A'^{(S_2)} (e^{-M't} + e^{-M'(T-t)}) + \dots, \end{aligned} \quad (4.10)$$

where a prime denotes a standard excited state of the same parity and a tilde denotes the mass or amplitude of an opposite-parity state. The oscillating behavior is visible throughout the entire lattice temporal extent, and must be included in fits to extract the ground-state mass and amplitudes.

We then obtain the renormalized decay amplitude in lattice units from the ratio

$$a^{3/2} \phi_H = \sqrt{2} \frac{Z_{A_{Qq}^4} A_{\Phi}^{(S)}}{A^{(S)}}, \quad (4.11)$$

where $A_{\Phi}^{(S)}$ and $A^{(S)}$ are the amplitudes of the ground state exponentials defined in Eqs. (4.9) and (4.10), and the renormalization factor $Z_{A_{Qq}^4}$ is discussed in Sec. V.

B. Analysis I

Our primary analysis of two-point correlation functions $\Phi_2^{(S)}$ and $C_2^{(S_1 S_2)}$ —“Analysis I”—proceeds as follows. The amplitudes $A_{\Phi}^{(S)}$ and $A^{(S)}$ in Eq. (4.11) are determined from fits to multiple correlators using the full data correlation matrix. In Analysis I, we start by fitting combinations A, B, C and D in Table VI. We find combination A, which uses the axial-current correlator with a $1S$ smeared source and the pseudoscalar correlator with a $1S$ smeared source and sink, to be suitable. The extra complexity of combinations of three correlators (C and D) give little benefit, and the errors from combination A are somewhat smaller than those from combination B.

For fits to charm-light meson correlators, we include just one simple exponential (the desired state) and one oscillating exponential, which we call a “1+1 state fit”. We choose the minimum distance, t_{min} , such that contributions from excited states are small compared to our statistical errors. Because we fit two propagators simultaneously while imposing the constraint that the masses be equal, this is a six parameter fit: two amplitudes for each

TABLE VI. Combinations of two-point functions that can be used to extract $a^{3/2}\phi_H$. All combinations of two and three correlators are shown. Additional combinations of four or more correlators are not enumerated.

two-point function	fit combination					
	A	B	C	D	E	F
$\Phi_2^{(1S)}(t)$	•		•	•	•	•
$\Phi_2^{(\delta)}(t)$		•	•	•	•	•
$C_2^{(1S,1S)}(t)$	•				•	•
$C_2^{(\delta,\delta)}(t)$		•			•	
$C_2^{(\delta,1S)}(t)$			•			•
$C_2^{(1S,\delta)}(t)$				•		

propagator and a common mass for each of the simple and oscillating exponentials. To help stabilize the fit, the amplitudes and mass of the oscillating state are weakly constrained by Gaussian priors, which are incorporated as additional terms in χ^2 in the fitting procedure [68, 69]. The central values for these priors are determined by a trial fit where the prior for the opposite parity mass is set to 500 ± 250 MeV above the ground state mass and the amplitudes are unconstrained. Then the jackknife fits use central values for the opposite parity state amplitudes and mass determined by the trial fit, with widths (Gaussian) that are typically three to ten times the error estimates on these parameters, so in the end the priors make a negligible contribution to χ^2 . (Although 500 MeV is a reasonable guess for the mass gap to the first excited state of the meson, we actually expect that this excited state in the fit approximates the contributions of a number of physical states, likely including both single and multiparticle channels.) Empirically, the width of the prior is made narrow enough to insure that the fits converge to sensible values. We propagate the uncertainties in the correlator fits to the subsequent chiral-continuum extrapolation with a jackknife procedure. In the jackknife resamples, we center the priors at the values found in the fit to the full ensemble, again with widths that are typically three to ten times the error estimates on these parameters.

The bottom meson correlators fall off much more rapidly with t , so it is difficult to take a large enough minimum distance to insure that excited state contributions are negligible. Therefore we use a fit with two simple exponentials and one oscillating exponential or a “2+1 state fit”. The mass of this excited state is also weakly constrained by priors in the same way that the opposite parity mass is, except that the width of the prior on the excited state mass is set to 200 MeV.

Figure 1 shows the heavy-light pseudoscalar mass as a function of the minimum time used in the fit. The left-hand plots show sample fits to bottom correlators, while the right-hand plots show sample fits to charm correlators. We select fitting ranges to give reasonable fits for all sea-quark ensembles and all valence-quark masses. We quantify the goodness-of-fit with the “ p value” [51], which is the probability that a fit with this number of degrees of freedom would have a χ^2 larger than this value. Table VII gives the fit ranges for charm-light and bottom-light correlators on the three lattice spacings, both for the fits used for the central values and for alternate fits used in estimating systematic errors from choices of fit parameters. The meson masses, $a^{3/2}\phi_H$ values, and p values for the data set used in

TABLE VII. Numbers of states and time ranges used in two-point Analysis I. In the number of states, “1+1” means one simple exponential and one oscillating state (opposite parity). The fits in columns two through five were used for the central values, while the fits in columns six through nine were used in estimating systematic errors from the choice of fit ranges (see Sec. VIIC).

$\approx a$ [fm]	central fits				alternate fits			
	charm		bottom		charm		bottom	
	n_{states}	t range	n_{states}	t range	n_{states}	t range	n_{states}	t range
0.15	1+1	11–23	2+1	4–20	1+1	12–23	1+1	9–20
0.12	1+1	14–31	2+1	5–22	1+1	16–31	1+1	12–22
0.09	1+1	21–47	2+1	7–30	1+1	23–47	1+1	16–30

Analysis I are tabulated in Appendix B.

The decay amplitude $a^{3/2}\phi_H$ is highly correlated among different light valence-quark masses on the same ensemble. To propagate the correlations among the different valence masses to the subsequent chiral-continuum extrapolation, in Sec. VI, we use a single-elimination jackknife procedure to estimate the covariance matrix of $a^{3/2}\phi_H$ for the selected valence quark masses. This is done by computing the covariance matrix of the single elimination jackknife samples, and multiplying by $(N - 1)^2$, where N is the number of configurations in the ensemble. In fact, when all valence quark masses are kept, the covariance matrices are close enough to singular to be unmanageable. This reflects the fact that the correlators for intermediate valence masses can be very accurately predicted from the correlators for nearby masses, so some of the correlators provide very little new information. Therefore, we omit some valence quark masses, using only those set in bold in Table II.

We use a single elimination jackknife rather than an omit- J jackknife because a large number of samples are needed to compute a reliable covariance matrix. Successive configurations in the ensemble are not independent, however, so we must take autocorrelations into account. We do so by repeating the calculation after first blocking the data by a factor of four. (This block size of four is determined from tests on the $a \approx 0.12$ fm lattices using fit Analysis II, for which it gives a reasonable compromise between suppressing autocorrelations and leaving enough data points for the statistical analysis.) We then compute, for each valence-quark mass i , the ratio R_i of the diagonal element of the covariance matrix with a block size of four to the same element of the unblocked covariance matrix:

$$R_i = \sigma_{ii}^{(4)} / \sigma_{ii}, \quad (4.12)$$

where the superscript denotes the block size. The rescaled covariance matrix for $a^{3/2}\phi_H$ is given by

$$C_{ij}^{(4)} = C_{ij} \sqrt{R_i R_j}, \quad (4.13)$$

which preserves the eigenvalue structure of the covariance matrix, whereas simply using the covariance matrix of the blocked data would be more likely to produce spurious small eigenvalues. The rescaling factors R_i themselves have errors, and in many cases turn out to be less than one. In such cases, we do not replace the R_i by one, despite the fact that this would likely be a better estimate of the individual R_i . Doing so would yield a covariance matrix with a bias toward larger errors, and could produce misleading estimates of goodness-of-fit in the later analysis.

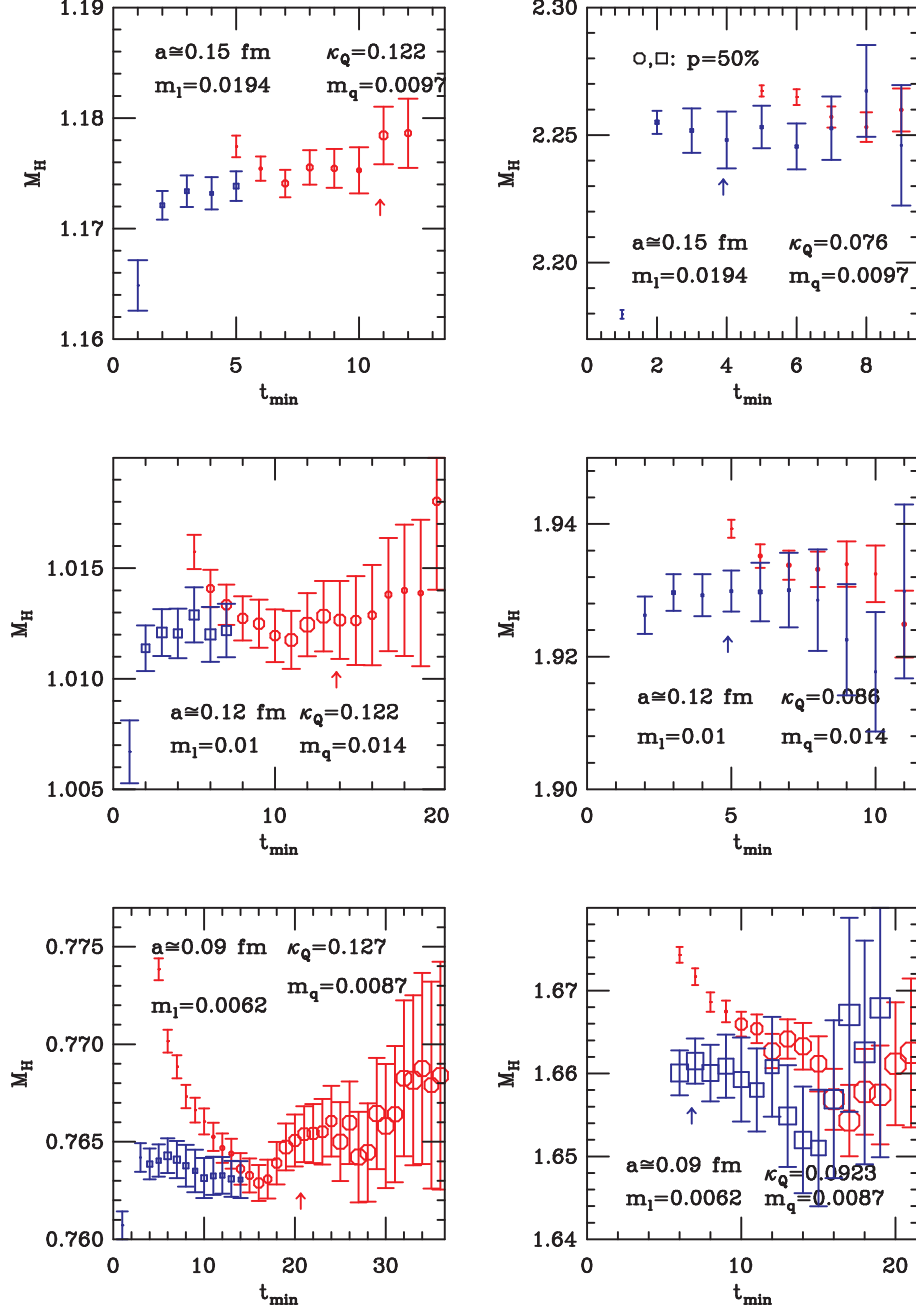


FIG. 1. Ground-state rest mass M_H versus minimum distance $t_{\min}$ included in the fit. For each lattice spacing, we show an ensemble with the dynamical light-quark mass m_l in the middle of the range. Similarly, we show correlators with a valence quark mass m_V in the center of the ranges used. The top two panels are at $a \approx 0.15$ fm, the middle two at $a \approx 0.12$ fm and the bottom two at $a \approx 0.09$ fm. In each row the left panel shows results for charm and the right-panel shows results for bottom. The size of each plot symbol is proportional to the p value (confidence level) of the fit, with the symbol size in the legends of the upper right panel corresponding to $p = 50\%$. The red octagons are for fits including one state of each parity ("1+1 fits") and the blue squares are for fits including an excited state of the same parity as the ground state ("2+1 fits"). In each panel, the arrow indicates the fit that is used in Sec. VI.

Finally, we combine the covariance matrices from all of the individual ensembles into larger covariance matrices, one each for the charm and bottom $a^{3/2}\phi_H$. Since different ensembles are statistically independent, these large covariance matrices are block diagonal, with each block containing the correlations among different light valence-quark masses on a single sea-quark ensemble.

C. Analysis II

Analysis II is a second, independent analysis of the two-point correlators that uses the bootstrap method to propagate correlated errors from the two-point analysis through to the chiral extrapolations. In Analysis II, we block average the two-point correlator data over four sequential configurations (which themselves are spaced by more than four trajectories) before the analysis. In the bootstrap procedure, we resample the data (with replacement), taking the number of sampled configurations to be equal to the number of blocked configurations in each bootstrap ensemble. For each bootstrap ensemble, we recompute the covariance matrix. During the bootstrap process, we randomly draw from a gaussian distribution new prior mean values of each constrained parameter belonging to an excited state while keeping the widths fixed. The ground state parameters are given loose priors so that the fitted values are determined by the data. To help stabilize the fits, the ground state prior means are not randomized in the bootstrap. Prior values for the energy splittings are taken from a chiral quark model calculation for the D and B meson systems [75]. Prior widths are taken to be about 200 MeV for excited states. Excited state amplitudes $\log(A^{(S)})$ have a prior width $\sigma_{\log A} = 2$.

On each gauge ensemble, the same sequence of gauge resamplings is taken for all valence m_q to preserve correlations among $a^{3/2}\phi_H$ values. Our final results are based upon 4,000 bootstrap replications of the data. We use the central values of $a^{3/2}\phi_H$ from the fits to the entire ensemble in the chiral-continuum extrapolation, and use the bootstrap values to obtain the covariance matrix.

To optimize the determination of $a^{3/2}\phi_H$, we compare simultaneous fits of up to six two-point functions; the various combinations of up to four functions are listed in Table VI. At a minimum, one axial-current correlator must be paired with one propagator (combinations A or B in Table VI) to extract $a^{3/2}\phi_H$. Combination A, using smeared operators, is used in Analysis I, described above. Because fits of four or more two-point functions over a wide time range can lead to a poorly determined data covariance matrix having large rank relative to the number of available configurations, we focus on combinations having two or three correlators. Unlike combination A, combination B does not take advantage of smeared sources and the ratio does not show convincing plateaus over the range of times with decent signal to noise. Comparing combination C to D, the smeared source in C is less noisy than the smeared sink in D.

Given these considerations, for fits to charm correlators, we use two-point function combination C to obtain $a^{3/2}\phi_H$ which uses both of the axial current functions. We look for stability of the ground-state mass and amplitude when varying t_{min} , t_{max} , and the number of excited states included in the fit. We also compare fit results from other combinations of correlators to check that we have isolated the correct ground-state energy and matrix element. Our final results come from fits accounting for two pseudoscalar states and two (oscillating) opposite-parity states.

For fits to bottom correlators, we use combination B for our final results; this is the same

set used in Analysis I. Combination C gives fits with rather low confidence levels for the B meson and tends to result in larger errors for $a^{3/2}\phi_H$. Again, we examine fits varying the time range; we also try fits with up to three pseudoscalar states plus three oscillating opposite parity states. We use these fits and fits to alternate combinations of two-point correlators as a consistency check.

The fit results from the two different analyses are consistent with each other for most cases, but there are a few cases where they differ by a standard deviation or more (see Figure 11). The $a^{3/2}\phi_H$ results from the two analyses are propagated through the chiral-continuum extrapolations in Secs. VIB and VIC. The resulting differences in the extrapolated results in turn provide the basis for our systematic error analysis due to fit choices given in Sec. VIIC.

V. HEAVY-LIGHT CURRENT MATCHING

In this section, we discuss in more detail the ingredients of Eq. (2.5), which allow a “mostly nonperturbative” matching procedure [42].

A. Perturbative calculation of $\rho_{A_{Qq}^4}$

The perturbative expansion of $\rho_{A_{Qq}^4}$ can be written as

$$\rho_{A_{Qq}^4} = 1 + \alpha_s(q^*)\rho_{A^4}^{[1]}(m_Q a, m_q a) + \dots \quad (5.1)$$

where α_s is the strong coupling and $\rho_{A^4}^{[1]}$ is the one-loop coefficient. The one-loop coefficient is calculated in Ref. [43] using lattice perturbation theory, where we see explicitly that $\rho_{A^4}^{[1]}$ is small because most of the one-loop corrections cancel. The self-energy contributions cancel exactly (to all orders, in fact), and, in practice, we are in a region where $\rho_{A^4}^{[1]}(m_Q a, m_q a)$, viewed as a function of $m_Q a$, has two zeroes. Therefore the renormalization factor $\rho_{A_{Qq}^4}$ is close to unity for both bottom and charm.

The perturbative calculation of $\rho_{A_{Qq}^4}$ in Eq. (5.1) proceeds as follows. We use $\alpha_s(q^*)$ defined in the V scheme [76] as determined in Ref. [77], and take $q^* = 2/a$, which is close to the optimal choice of Refs. [76, 78] for a wide range of quark masses. The one-loop coefficients $\rho_{A^4}^{[1]}$ are computed for light-quark masses $am_q = 0.001, 0.01, 0.04$ to cover the range used in this analysis. From these we obtain $\rho_{A_{Qq}^4}$ at other light-quark masses by linear interpolation in am_q . For illustration, Table VIII lists $\rho_{A_{bq}^4}$ and $\rho_{A_{cq}^4}$ evaluated at the light valence mass $am_q = 0.01$ for the eleven sea-quark ensembles used in this work. Note that the sea-quark mass dependence is indirect, via the plaquette used to determine $\alpha_s(q^*)$. The dependence on the light-quark mass in the current is very mild: for bottom, $\rho_{A_{bq}^4}$ changes with am_q by 0.07–0.2%, depending on lattice spacing, and for charm, $\rho_{A_{cq}^4}$ changes by around 0.1%. On the fine ensembles, the am_q dependence is almost as large as the total one-loop correction because the overall cancellation, especially in $\rho_{A_{cq}^4}$, is so fortuitously good.

TABLE VIII. The perturbative correction factor $\rho_{A_{Qq}^4}$ for the heavy-light current A^4 at the simulated charm and bottom heavy quark κ values given in Table III and at $am_q = 0.01$ for the different sea-quark ensembles. The statistical errors associated with the numerical integration are negligible.

$\approx a$ [fm]	am_l/am_h	$\rho_{A_{bq}^4}$	$\rho_{A_{cq}^4}$
0.09	0.0031/0.031	1.0026	1.0000
	0.0062/0.031	1.0026	1.0000
	0.0124/0.031	1.0026	1.0000
0.12	0.005/0.05	1.0081	0.9959
	0.007/0.05	1.0081	0.9959
	0.010/0.05	1.0081	0.9959
	0.020/0.05	1.0080	0.9960
	0.030/0.05	1.0079	0.9961
0.15	0.0097/0.0484	1.0270	0.9937
	0.0194/0.0484	1.0267	0.9938
	0.0290/0.0484	1.0265	0.9938

B. Nonperturbative computation of $Z_{V_{qq}^4}$ and $Z_{V_{Qq}^4}$

The nonperturbative part of the matching factor $Z_{A_{Qq}^4}$ is obtained from the temporal components of the clover-clover and staggered-staggered vector currents. At zero-momentum transfer, the (correctly normalized) vector current simply counts flavor-number, so it is possible to obtain Z_{V^4} nonperturbatively for any discretization and any mass [42].

For the staggered-staggered current, we compute

$$C_3^{(S_1 S_2)}(t_2, 0, t_1) = \sum_{ab} \sum_{\mathbf{x}, \mathbf{y}} \left\langle \mathcal{O}_a^{(S_1)}(t_2, \mathbf{y}) V_{ab}^4(0) \mathcal{O}_b^{(S_2)\dagger}(t_1, \mathbf{x}) \right\rangle, \quad (5.2)$$

where, as in Eq. (4.5), $\mathcal{O}_a^{(S)}$ is a smeared or local clover-staggered meson operator with mass chosen to optimize the signal, and

$$V_{ab}^4(x) = \bar{\chi}(x) [\Omega^\dagger(x) \gamma^4 \Omega(x)]_{ab} \chi(x) \quad (5.3)$$

is the temporal component of the staggered-staggered vector current. The three-point functions C_3 are computed from the same staggered quarks used for the clover-staggered two point functions. The staggered quark is transformed into an improved naive quark by applying the Ω matrix; this naive quark at time t_1 is then used as the source term when computing the charm propagator. We smear the source at t_1 so that $S_1 = S_2$.

We compute $Z_{V_{qq}^4}$ using a D_q meson [cf. Eq. (4.5)], which provides a good signal. The three-point function $C_3^{(S_1 S_2)}(t_2, 0, t_1)$ contains states of both the desired and the opposite parity, with the latter carrying oscillating $(-1)^t$ dependence. We construct $C_3^{(S_1 S_2)}(t_2, 0, t_1)$ with local sources $S_1 = S_2 = \delta$ and compute it at multiple even and odd values of t_1 and t_2 in order to disentangle the ground-state amplitude from the other contributions.

TABLE IX. Light-light vector current renormalization factor $Z_{V_{qq}^4}$. Values in bold are used in computing the heavy-light current renormalizations. With our conventions, the tree-level value of $Z_{V_{qq}^4}$ is 2. A colon is used to represent the range of time values included in the fit.

$\approx a$ [fm]	am_l/am_h	n_{conf}	$-t_1$	t_2	am_q	$Z_{V_{qq}^4}$
0.09	0.0124/0.031	518	23:12	11:13	0.0272	1.868(49)
			23:12	11:13	0.0124	1.883(69)
0.12	0.01/0.05	592	15:9	7:11	0.03	1.853(45)
	0.007/0.05	523	20:7	7:12	0.03	1.882(56)
0.15	0.0097/0.0484	631	20:5	4:12	0.0484	1.704(34)
			20:5	4:12	0.029	1.709(40)
			20:5	4:12	0.0242	1.711(42)
			20:5	4:12	0.0194	1.707(45)
			20:5	4:12	0.0097	1.662(55)

Within the time range $t_1 < 0 < t_2$ and in the limit of large separations, $|t_1|, t_2 \gg a$,

$$\begin{aligned}
C_3^{(\delta, \delta)}(t_2, 0, t_1) &= Z_{V_{qq}^4}^{-1} A^2 \exp(-E(t_2 - t_1)) \\
&+ Z' AB \left[(-1)^{t_1} \exp(E't_1 - Et_2) + (-1)^{t_2} \exp(Et_1 - E't_2) \right] \\
&+ Z'' B^2 (-1)^{(t_1+t_2)} \exp(-E'(t_2 - t_1)) + \dots,
\end{aligned} \tag{5.4}$$

neglecting contributions from excited states. We extract $Z_{V_{qq}^4}$ from a minimum χ^2 fit to the three-point function using the right-hand side of Eq. (5.4) as the model function. The fit is linear in the free parameters $Z_{V_{qq}^4}^{-1}$, Z'' and Z' , while we fix the ground-state energies E and E' , and the operator overlaps A and B to the values determined by fitting the two-point function $C_2^{(\delta)}(t, \mathbf{0})$. We use a single-elimination jackknife procedure to compute the data covariance matrix.

Table IX presents our results for $Z_{V_{qq}^4}$ on the ensembles used in this work. The three-point functions for the $Z_{V_{qq}^4}$ calculation are generated at a single source time, $t_{\text{src}} = 0$ (instead of the four used for two-point functions $\Phi_2^{(S)}$ and $C_2^{(S_1 S_2)}$). At $a \approx 0.12$ fm we have results at two values of the sea quark masses which are consistent within errors. At $a \approx 0.09$ and 0.15 fm we have results for several values of m_q . We do not see evidence for a dependence upon m_q with current statistics. The errors, however, increase at smaller quark mass. Hence, we use the $Z_{V_{qq}^4}$ corresponding to $m_q \sim m_s$ in Eq. (4.11). In the table, they are set in **bold**.

For the clover-clover current, we compute

$$\tilde{C}_3^{(S_1 S_2)}(t_2, t_1, 0) = \sum_{\mathbf{x}, \mathbf{y}} \left\langle \tilde{\mathcal{O}}^{(S_1)\dagger}(t_2, \mathbf{y}) V_{QQ}^4(t_1, \mathbf{x}) \tilde{\mathcal{O}}^{(S_2)}(0) \right\rangle, \tag{5.5}$$

where

$$V_{QQ}^4(x) = \bar{\Psi}(x) \gamma^4 \Psi(x) \tag{5.6}$$

is the temporal component of the (rotated) clover-clover vector current. The clover-clover bilinear

$$\tilde{\mathcal{O}}^{(S)}(x) = \sum_y \bar{\psi}(y) S(x, y) \gamma^5 s(x) \tag{5.7}$$

TABLE X. Heavy-heavy vector current renormalization factor $Z_{V_{QQ}^4}$ computed at several κ values, covering the charm and bottom quark masses, for three lattice spacings.

$\approx a$ [fm]	am_l/am_h	$n_{\text{conf}} \times n_{\text{src}}$	κ_Q	$Z_{V_{QQ}^4}$
0.09	0.0062/0.031	1912×2	0.1283	0.2749(4)
			0.127	0.2830(4)
			0.110	0.3856(6)
			0.0950	0.4730(8)
			0.0931	0.4840(9)
0.12	0.007/0.05	2110×2	0.124	0.2899(4)
			0.122	0.3028(4)
			0.116	0.3410(5)
			0.098	0.4507(7)
			0.086	0.5209(10)
0.15	0.0194/0.0484	631×2	0.122	0.3195(14)
			0.118	0.3440(16)
			0.088	0.5195(48)
			0.076	0.5898(81)

consists of a heavy-quark field corresponding to charm or bottom, as the case may be, and a light clover-quark field s with mass chosen to provide a good signal. At large time separations, these three-point functions are proportional to $Z_{V_{QQ}^4}^{-1}$, with the proportionality coming from

$$\tilde{C}_2^{(S_1 S_2)}(t) = \sum_{\mathbf{x}} \left\langle \tilde{\mathcal{O}}^{(S_1)\dagger}(t, \mathbf{x}) \tilde{\mathcal{O}}^{(S_2)}(0) \right\rangle. \quad (5.8)$$

We compute $Z_{V_{QQ}^4}$ using a $\bar{Q}s$ meson, where the strange quark is simulated with the clover action to circumvent oscillating opposite-parity states [*cf.* Eq. (5.7)]. We restrict our calculation of $\tilde{C}_{2,3}$ to $S = S_1 = S_2$ using both local and 1S smearing functions. The function $\tilde{C}_2$ combines a local-local clover quark with mass around m_s and a heavy clover quark propagator with source and sink S . The function $\tilde{C}_3$ requires the same heavy- and light-quark propagators as needed in $\tilde{C}_2$. An additional heavy-quark propagator originating from t_2 has as its source the light quark propagator restricted to t_2 , multiplied by γ_5 and convolved with smearing function S .

In Eq. (5.7), we use a random color wall source with three dilutions for both the heavy and light spectator quarks that originate from $t = 0$. We generate two- and three-point functions for both local-local and smeared-smeared source-sink combinations where the smearing is applied to the heavy quark. We compute the 2- and 3-point functions at several values of κ spanning a range from around the charm quark to the bottom quark. We determine $Z_{V_{QQ}^4}$ from a fit to the plateaus in the jackknifed ratio of the three-point and two-point functions. Our results are summarized in Table X.

In order to properly normalize the derivative $d\phi/d\kappa_Q$ (see Eq. (3.5)), we need values of $Z_{V_{QQ}^4}$ at κ values other than those used in the $Z_{V_{QQ}^4}$ simulations. We therefore fit the

TABLE XI. Heavy-heavy vector current renormalization factor $Z_{V_{QQ}^4}$ corresponding to the charm and bottom κ_{sim} values used in the decay constant simulations.

$\approx a$ [fm]	charm		bottom	
	κ_Q	$Z_{V_{QQ}^4}$	κ_Q	$Z_{V_{QQ}^4}$
0.09	0.127	0.2829(4)	0.0923	0.4891(9)
0.12	0.122	0.3029(4)	0.086	0.5216(10)
0.15	0.122	0.3199(14)	0.076	0.5868(81)

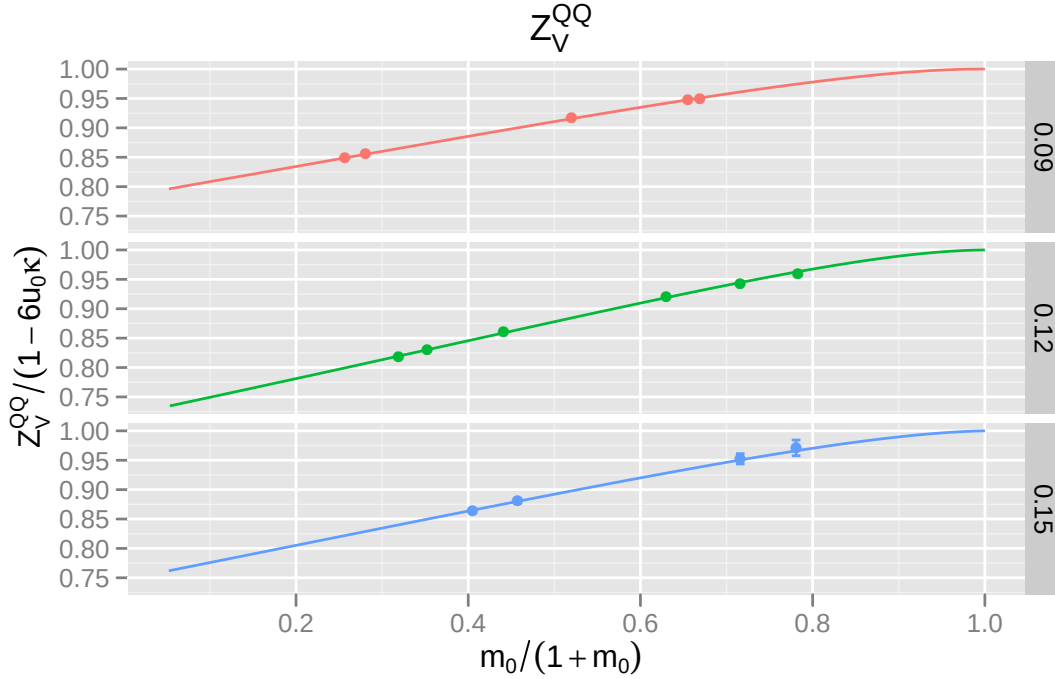


FIG. 2. Plot of $Z_{V_{QQ}^4}/(1 - 6u_0\kappa)$ vs. $m_0a/(1 + m_0a)$ for the three lattice spacings.

simulation results to the interpolating quartic polynomial

$$Z_{V_{QQ}^4}(\kappa) = 1 + \sum_{j=1}^4 c_j \kappa^j \quad (5.9)$$

which reproduces the infinite mass limit $Z_{V_{QQ}^4} \rightarrow 1$. Our codes employ the hopping parameter version of the action; so, at tree level $c_1 = -6u_0$ and for $j > 1$, $c_j = 0$. We constrain the interpolation parameters to the tree-level values taking $\sigma_j = 4$ as the widths. Table XI shows values for $Z_{V_{QQ}^4}$ interpolated to the nominal charm and bottom κ_{sim} used in our decay constant runs. Figure 2 plots the data in Table X together with the interpolation of Eq. (5.9). To aid perturbative intuition, the values of $Z_{V_{QQ}^4}$ in the figure are scaled by the tree-level expression $1 - 6u_0\kappa$; the relation between κ and $m_0a/(1 + m_0a)$ can be inferred from Eq. (4.4).

VI. CHIRAL AND CONTINUUM EXTRAPOLATION

In this section, we present the combined chiral and continuum extrapolations used to obtain the physical values of the $B_{(s)}$ and $D_{(s)}$ meson decay constants. We first discuss the use of $SU(3)$ chiral perturbation theory for heavy-light mesons in Sec. VIA, giving the formulas used for the chiral fits and describing our method for incorporating heavy-quark and light-quark discretization effects into the extrapolation. We then show the chiral fits for the D system in Sec. VIB, and for the B system in Sec. VIC.

A. Chiral Perturbation Theory framework

The errors introduced by the chiral and (light-quark) continuum extrapolations are controlled with rooted staggered chiral perturbation theory (rS χ PT) [22, 23] applied to heavy-light mesons. In Ref. [39], the heavy-light decay constant was calculated to one-loop in rS χ PT at leading order in the heavy-quark expansion $[(1/M_H)^0]$, where M_H is a generic heavy-light meson mass. A replica trick is used in rS χ PT to take into account the effect of the fourth root of the staggered determinant [15, 21].

In addition to using the form calculated in Ref. [39], we also use a chiral fit form that includes, in the loops, the effects of hyperfine splittings (*e.g.*, $M_B^* - M_B$) and flavor splittings (*e.g.*, $M_{B_s} - M_B$). These splittings are ~ 100 MeV, and so not much smaller than M_π , despite the fact that they are formally of order $1/M_H$. Since the lightest pseudoscalar meson masses in our simulations are ~ 225 MeV, it is not immediately obvious that including the splittings is necessary or useful. Their inclusion is motivated, first of all, by the observation of Arndt and Lin [79] that finite-volume effects in the one-loop diagrams can be substantially larger with the splittings present. This is mainly due to the fact that accidental cancellations in finite volume effects between different diagrams at $(1/M_H)^0$ disappear once splittings are included. As described below, it is not difficult to include the splitting effects into the calculation of Ref. [39]. We also discuss the extent to which including the splittings, but not other effects that could occur at order $1/M_H$, is a systematic approximation. In practice, we do fits both including and omitting the splittings, and use the difference as one estimate of the chiral extrapolation error. For central values, we include the splittings, because this yields a more conservative estimate of finite-volume effects.

With staggered quarks, the (squared) pseudoscalar meson masses are

$$M_{ab,\xi}^2 = B_0(m_a + m_b) + a^2 \Delta_\xi, \quad (6.1)$$

where m_a and m_b are quark masses, B_0 is a parameter of χ PT, and the representation of the meson under the taste symmetry group is labeled by $\xi = P, A, T, V, I$ [22]. The exact non-singlet chiral symmetry of staggered quarks as $m_a, m_b \rightarrow 0$ ensures that $\Delta_P = 0$. All of these pseudoscalars appear in the “pion” cloud around the heavy-light meson in the simulation, and all of them therefore affect the decay constant.

Working at leading order $[(1/M_H)^0]$ in the heavy-quark expansion and at one loop, or next-to-leading order (NLO), in the chiral expansion, the rS χ PT expression for the decay

constant with light valence quark q takes the form [39]

$$\begin{aligned} \phi_{H_q} = \phi_H^0 & \left[1 + \frac{1}{16\pi^2 f^2} \frac{1 + 3g_\pi^2}{2} \left\{ -\frac{1}{16} \sum_{e,\xi} \ell(M_{eq,\xi}^2) \right. \right. \\ & - \frac{1}{3} \sum_{j \in \mathcal{M}_I^{(2,q)}} \frac{\partial}{\partial M_{Q,I}^2} \left[R_j^{[2,2]}(\mathcal{M}_I^{(2,q)}; \mu_I^{(2)}) \ell(M_j^2) \right] \\ & - \left(a^2 \delta'_V \sum_{j \in \hat{\mathcal{M}}_V^{(3,q)}} \frac{\partial}{\partial M_{Q,V}^2} \left[R_j^{[3,2]}(\hat{\mathcal{M}}_V^{(3,q)}; \mu_V^{(2)}) \ell(M_j^2) \right] + [V \rightarrow A] \right) \Bigg\} \\ & \left. + p(m_q, m_l, m_h, a^2) \right], \end{aligned} \quad (6.2)$$

where m_q is the light valence-quark mass, e runs over the sea quarks, the lighter two of which have masses m_l , and the heavier, m_h .¹ The parameter ϕ_H^0 is independent of the light masses, and p is an analytic function. We fit the charm and bottom systems separately, so ϕ_H^0 depends, in practice, on the heavy-quark mass. The meson mass $M_{Q,\xi}$ is similar to $M_{ab,\xi}$ in Eq. (6.1), but constructed from a valence quark-antiquark, $q\bar{q}$. The light-meson decay constant $f \approx f_\pi \cong 130.4$ MeV and the H - H^* - π coupling g_π controls the size of the one-loop effects. Taste-violating hairpin diagrams, which arise only at non-zero lattice spacing, are parameterized by δ'_A and δ'_V . The residue functions $R_j^{[n,k]}(\{M\}, \{\mu\})$ are defined in Ref. [23]. Chiral logarithms are written in terms of the functions $\ell(M^2)$ [80]:

$$\ell(M^2) = M^2 \ln \frac{M^2}{\Lambda_\chi^2} \quad [\text{infinite volume}], \quad (6.3)$$

$$\ell(M^2) = M^2 \left(\ln \frac{M^2}{\Lambda_\chi^2} + \delta_1(ML) \right) \quad [\text{spatial volume } L^3], \quad (6.4)$$

$$\delta_1(ML) \equiv \frac{4}{ML} \sum_{\mathbf{r} \neq \mathbf{0}} \frac{K_1(|\mathbf{r}|ML)}{|\mathbf{r}|}. \quad (6.5)$$

Here Λ_χ is the chiral scale, K_1 the Bessel function of imaginary argument, and $\mathbf{r}$ any non-zero three-vector with integer components. The mass sets in the residue functions of Eq. (6.2) are

$$\mu^{(2)} = \{M_U^2, M_S^2\}, \quad (6.6)$$

$$\mathcal{M}^{(2,q)} = \{M_Q^2, M_\eta^2\}, \quad (6.7)$$

$$\hat{\mathcal{M}}^{(3,q)} = \{M_Q^2, M_\eta^2, M_{\eta'}^2\}, \quad (6.8)$$

where M_U (M_S) is the mass of the pseudoscalar $l\bar{l}$ ($h\bar{h}$) meson.

The salient feature of the chiral extrapolation of ϕ_{H_q} is that the chiral logs have a characteristic curvature as $m_q \rightarrow 0$ [81]. At non-zero lattice spacing, the presence of the additive splittings $a^2 \Delta_\xi$ in the meson masses reduces the curvature of the chiral logarithms. The characteristic curvature returns, however, as the continuum limit is approached.

¹ The physical values of the average up-down quark mass and of the strange-quark mass are denoted by $\hat{m} = (m_u + m_d)/2$ and m_s , respectively.

To combine data from several lattice spacings into one chiral extrapolation, it is necessary to convert lattice units to (some sort of) physical units. As mentioned in Sec. III A, we convert in two steps, first by canceling lattice units with the appropriate power of r_1/a . In particular, pseudoscalar meson masses [cf. Eq. (6.1)] become $r_1^2 M_{ab,\xi}^2 = (r_1/a)^2 (a M_{ab,\xi})^2$, and the decay constant [cf. Eq. (6.2)] becomes $r_1^{3/2} \phi_H = (r_1/a)^{3/2} (a^{3/2} \phi_H)$, with $a^{3/2} \phi_H$ determined from Analyses I or II (cf. Sec. IV). Strictly speaking, one must take the quark mass dependence of r_1 into account, either separately or by modifying the right-hand side of Eq. (6.2) accordingly. At the present level of accuracy, we ignore this subtlety, canceling units ensemble-by-ensemble with the computed r_1/a . Since r_1 is expected to depend smoothly on m_l and m_h , we are unlikely to introduce an uncontrolled error into the extrapolated decay constants. (After completing the chiral-continuum extrapolation in r_1 units, we then use $r_1 = 0.3117(22)$ fm (cf. Sec. III A) to convert to MeV.)

To quantify the size of NLO (and higher) corrections to χ PT, it is useful to define dimensionless parameters x_q , x_l and x_h proportional to the quark masses m_q , m_l and m_h :

$$x_{q,l,h} \equiv \frac{(r_1 B_0)(r_1/a)(2am_{q,l,h})}{8\pi^2 f_\pi^2 r_1^2}.$$

Since the splittings $a^2 \Delta_\xi$ are added to the quark mass terms in Eq. (6.1), it is similarly useful to define

$$x_{\Delta_\xi} \equiv \frac{r_1^2 a^2 \Delta_\xi}{8\pi^2 f_\pi^2 r_1^2}, \quad (6.9)$$

$$x_{\bar{\Delta}} \equiv \frac{r_1^2 a^2 \bar{\Delta}}{8\pi^2 f_\pi^2 r_1^2}, \quad (6.10)$$

where $\bar{\Delta}$ is the average pion splitting

$$\bar{\Delta} = \frac{1}{16}(\Delta_P + 4\Delta_A + 6\Delta_T + 4\Delta_V + \Delta_I). \quad (6.11)$$

The x_i are in “natural” units for χ PT, in the sense that one expects that chiral corrections, when written as series in the x_i , have coefficients [or low-energy constants (LECs)] that are of order 1.

We then take the analytic function p in Eq. (6.2) to have the following form at NLO

$$L_{\text{val}}(x_q + x_{\Delta_{\text{val}}}) + L_{\text{sea}}(2x_l + x_h + 3x_{\Delta_{\text{sea}}}) + L_a \frac{a^2}{16\pi^2 f_\pi^2 r_1^4}, \quad (6.12)$$

where L_{val} , L_{sea} and L_a are quark-mass-independent LECs that we fit from our data, and we define

$$x_{\Delta_{\text{val}}} \equiv \frac{9}{5}x_{\bar{\Delta}} - \frac{4}{5}x_{\Delta_I}, \quad (6.13)$$

$$x_{\Delta_{\text{sea}}} \equiv \frac{9}{11}x_{\bar{\Delta}} + \frac{2}{11}x_{\Delta_I}, \quad (6.14)$$

The low-energy constants L_{val} , L_{sea} and L_a depend implicitly on the chiral scale Λ_χ , so that the complete expression, Eq. (6.2), is independent of Λ_χ . As in Ref. [39], we choose to include the a^2 dependent terms $x_{\Delta_{\text{sea}}}$ and $x_{\Delta_{\text{val}}}$ in the coefficients of L_{val} and L_{sea} so that

these coefficients represent those combinations of meson masses that arise naturally under a change of Λ_χ in the chiral logarithms.

The LEC L_a arises from analytic taste-violating effects; it serves as a counterterm to absorb changes proportional to the taste-violating hairpins δ'_A and δ'_V under a change in chiral scale. As such, we take the a^2 coefficient of L_a in Eq. (6.12) to vary with lattice spacing like $x_{\Delta_{\text{val}}}$. As long as L_a then appears as an independent fit parameter, the introduction of the $x_{\Delta_{\text{sea}}}$ and $x_{\Delta_{\text{val}}}$ terms in the coefficients of L_{val} and L_{sea} in Eq. (6.12) has a negligible effect on the results from the chiral fits. However, we find that the introduction of these terms significantly reduces the magnitude of L_a ; in other words, most of the discretization error from the light quarks appears to be due to the a^2 dependence of the light meson masses in the chiral loops. We leave L_{val} , L_{sea} and L_a unconstrained in the fits that determine central values; their size is of $\mathcal{O}(1)$ as expected (and is in fact ≤ 0.6).

In the region of the strange-quark mass, the data for the decay constants show some curvature, and at least some quadratic terms in the quark masses (NNLO effects) must in general be added in order to obtain acceptable ($p > 0.01$) fits. There are four such LECs, giving a NNLO contribution to p of the form

$$Q_1 x_q^2 + Q_2 (2x_l + x_h)^2 + Q_3 x_q (2x_l + x_h) + Q_4 (2x_l^2 + x_h^2). \quad (6.15)$$

Fits omitting the Q_1 and Q_3 terms give poor confidence levels and are rejected; adding the Q_2 and Q_4 terms does not change the fit results much, but increases over-all errors by up to 30%. To be conservative, we include all four terms in fits for central values; other acceptable fits (for example, fixing Q_2 or Q_4 or both to zero) are included among the alternatives used to estimate the systematic error of the chiral extrapolation.

For the central-value fits, the Q_i are mildly constrained by Gaussian priors with central value 0 and width 0.5, since that is roughly the expected size in natural units. After fitting, the posterior values satisfy $|Q_i| \leq 0.5$, and Q_1 and Q_3 have errors ≈ 0.05 (much less than the prior width), indicating that they are constrained by the data. Q_2 and Q_4 have errors ~ 0.5 , indicating that they are largely constrained by the priors. Changing the prior widths for the Q_i to 1.0 has a negligible effect on central values and errors of the decay constants, although the posterior Q_2 and Q_4 typically increase in size and error, as expected.

While the chiral form introduced so far gives acceptable simultaneous fits to our data from all available lattice spacings, we still need to estimate the size of heavy-quark and generic light-quark discretization errors. Following the Bayesian approach advocated in Refs. [68, 69], we add constrained lattice-spacing-dependent terms to the fit function until the statistical errors of the results cease to increase appreciably. For the heavy quark, we take up to six such terms, $f_E(m_0 a)$, $f_X(m_0 a)$, $f_Y(m_0 a)$, $f_B(m_0 a)$, $f_3(m_0 a)$, and $f_2(m_0 a)$, where m_0 is the heavy quark bare mass. Details about the origin and form of these six functions are given in Appendix A. These functions estimate fractional (not absolute) errors, and as such are included within the square brackets in Eq. (6.2) (or its equivalent, Eq. (6.20) below). The first three are $\mathcal{O}(a^2)$ corrections and are added to the fit with coefficients $z_i (a\Lambda)^2$, $i \in \{E, X, Y\}$, where Λ is a scale characteristic of the heavy-quark expansion, and the z_i are parameters with prior value 0 and prior width 1 (for f_Y) or $\sqrt{2}$ (for f_E and f_X , since they each appear twice in the analysis of Appendix A). The next two terms are $\mathcal{O}(\alpha_s a)$ corrections, added with coefficients $z_i \alpha_s a \Lambda$, $i \in \{B, 3\}$, with z_i taken to have prior value 0 and prior width 1 (for f_B) or $\sqrt{2}$ (for f_3 , again because it appears twice). The final term arises from the propagation to the decay constants of heavy-quark errors in the tuning of the heavy-quark hopping parameter, κ . It comes in with coefficient $z_2 (a\Lambda)^3$, with z_2 having

prior value 0 and prior width 1. We take a large value $\Lambda = 700$ MeV, which provides conservatively wide priors, especially for the first five terms. Once one of each of the first two types of terms is added, the errors already reach $\sim 80\%$ of their values with all six added.

Similar terms representing generic light-quark errors, which are not automatically included in the fit function (unlike taste-violating terms), may also be added. With the asqtad staggered action, generic discretization effects are of $O(\alpha_s a^2)$. We allow the physical LECs ϕ_H^0 , L_{val} , L_{sea} , Q_1 , Q_2 , Q_3 , and Q_4 , to have small relative variations with lattice spacing with coefficients $C_i \alpha_s (a\Lambda)^2$, where i stands for any of the seven physical LECs, Λ is again taken to be 700 MeV, and the C_i have prior value 0 with prior width 1. This corresponds to a maximum of about a 3% difference for a given LEC between the $a \approx 0.12$ fm and the $a \approx 0.09$ fm ensembles. Once several heavy-quark discretization terms have been introduced, these light-quark terms further increase the total error of individual decay constants by less than 10%. However, the errors on the decay constant ratios f_{D_s}/f_{D^+} and f_{B_s}/f_{B^+} are significantly increased by light-quark discretization effects, because the heavy-quark effects on the ratios cancel to first approximation. For our central values, we include all six heavy-quark and all seven light-quark terms, so the total error from a given fit should estimate all (taste-conserving) discretization errors, as well as normal statistical effects. To estimate “heavy-quark” and “light-quark” discretization effects separately, we set to zero the light- or heavy-quark discretization terms, respectively, and then subtract the statistical errors in quadrature. Such separate errors are not relevant to any final results quoted below, but are included as separate lines in the error budget for informational purposes.

As mentioned above, our preferred fit form modifies Eq. (6.2) by including the effects of hyperfine and flavor splittings of the heavy-light mesons in one-loop diagrams. We now briefly describe how one may adjust the results of Ref. [39] to include these splittings. In Eq. (6.2), the contributions proportional to g_π^2 come from diagrams with internal H^* propagators, namely the left-hand diagrams in Fig. 5 of Ref. [39]. Contributions with no factor of g_π^2 come from diagrams with light-meson tadpoles, namely the right-hand diagrams in Fig. 5 of Ref. [39]. The latter have no internal heavy-light propagators, so are unaffected by any heavy-light splittings. The splittings in the former diagrams depend on whether the light-meson line is connected (Fig. 5a, left, of Ref. [39]), or disconnected (Fig. 5b, left). In the disconnected case, the H^* in the loop always has the same flavor (q) as the external H_q , so there is no flavor splitting between the two, only a hyperfine splitting. In the connected case, the H^* in the loop has the flavor of the virtual sea quark loop (which we labeled by e in Eq. (6.2)), so there is flavor splitting with the external H_q , in addition to the hyperfine splitting.

Let Δ^* be the (lowest-order) hyperfine splitting, and δ_{eq} be the flavor splitting between a heavy-light meson with light quark of flavor e and one of flavor q . At lowest order, δ_{eq} is proportional to the quark-mass difference (or light-meson squared mass difference), which can be written in terms of a parameter λ_1 :

$$\delta_{eq} \cong 2\lambda_1 B_0 (m_e - m_q) \cong \lambda_1 (M_E^2 - M_Q^2), \quad (6.16)$$

where M_E is the mass of an $e\bar{e}$ light meson. Here we have used the notation of Arndt and Lin [79] and included a factor of B_0 in the middle expression; B_0 is omitted in the notation of Ref. [82], Eq. (16), and of Ref. [39], Eq. (45).

By convention, the mass of the external H is removed in the heavy quark effective theory, so the mass shell is at $\mathbf{k} = \mathbf{0}$, where $\mathbf{k}$ is the external three-momentum. When there

is no splitting, the internal H^* has its pole at the same place, which makes the integrals particularly simple, giving the chiral log function $\ell(M^2)$, Eq. (6.3). If a splitting Δ is present, the integrals involve a significantly more complicated function, which we denote

$$J(M, \Delta) = (M^2 - 2\Delta^2) \log(M^2/\Lambda^2) + 2\Delta^2 - 4\Delta^2 F(M/\Delta) \quad [\text{infinite volume}]. \quad (6.17)$$

Here the function F is most simply expressed [83, 84]

$$F(1/x) = \begin{cases} -\frac{\sqrt{1-x^2}}{x} \left[\frac{\pi}{2} - \tan^{-1} \frac{x}{\sqrt{1-x^2}} \right], & \text{if } |x| \leq 1, \\ \frac{\sqrt{x^2-1}}{x} \ln(x + \sqrt{x^2-1}), & \text{if } |x| \geq 1, \end{cases} \quad (6.18)$$

which is valid for all x .

It is then straightforward to write down the generalization of Eq. (6.2) to include splittings. The basic rule is to replace

$$\ell(M^2) \rightarrow J(M, \Delta) \quad (6.19)$$

in the terms proportional to g_π^2 . It is not hard to show that $J(M, 0) = \ell(M^2)$, so this replacement is consistent with the original result neglecting the splittings. In making the replacements, one must choose the correct value of the splitting Δ in each term. As mentioned above, in terms that come from the diagram with a disconnected light-meson propagator, one must put $\Delta = \Delta^*$. But in terms that come from the diagram with a connected light-meson propagator, one must put $\Delta = \Delta^* + \delta_{eq}$, because the internal heavy-light meson is a H_e^* , while the external meson is an H_q . The result for the heavy-light meson decay amplitude including the splittings is then

$$\begin{aligned} \phi_{H_q} = \phi_H^0 & \left[1 + \frac{1}{16\pi^2 f^2} \frac{1}{2} \left\{ -\frac{1}{16} \sum_{e, \Xi} \ell(M_{eq, \Xi}^2) \right. \right. \\ & - \frac{1}{3} \sum_{j \in \mathcal{M}_I^{(2,x)}} \frac{\partial}{\partial M_{X,I}^2} \left[R_j^{[2,2]}(\mathcal{M}_I^{(2,x)}; \mu_I^{(2)}) \ell(M_j^2) \right] \\ & - \left(a^2 \delta'_V \sum_{j \in \hat{\mathcal{M}}_V^{(3,x)}} \frac{\partial}{\partial M_{X,V}^2} \left[R_j^{[3,2]}(\hat{\mathcal{M}}_V^{(3,x)}; \mu_V^{(2)}) \ell(M_j^2) \right] + [V \rightarrow A] \right) \\ & - 3g_\pi^2 \frac{1}{16} \sum_{e, \Xi} J(M_{eq, \Xi}, \Delta^* + \delta_{eq}) \\ & - g_\pi^2 \sum_{j \in \mathcal{M}_I^{(2,x)}} \frac{\partial}{\partial M_{X,I}^2} \left[R_j^{[2,2]}(\mathcal{M}_I^{(2,x)}; \mu_I^{(2)}) J(M_j, \Delta^*) \right] \\ & \left. - 3g_\pi^2 \left(a^2 \delta'_V \sum_{j \in \hat{\mathcal{M}}_V^{(3,x)}} \frac{\partial}{\partial M_{X,V}^2} \left[R_j^{[3,2]}(\hat{\mathcal{M}}_V^{(3,x)}; \mu_V^{(2)}) J(M_j, \Delta^*) \right] + [V \rightarrow A] \right) \right\} \\ & \left. + p(m_q, m_l, m_h, a^2) \right]. \quad (6.20) \end{aligned}$$

It is also straightforward to include finite-volume effects into Eq. (6.20). One simply replaces

$$J(M, \Delta) \rightarrow J(M, \Delta) + \delta J(M, \Delta, L), \quad (6.21)$$

where $\delta J(M, \Delta, L)$ is the finite-volume correction in a spatial volume L^3 . The correction can be written in terms of functions defined in Refs. [41, 79]:

$$\delta J(M, \Delta, L) = \frac{M^2}{3} \delta_1(ML) - 16\pi^2 \left[\frac{2\Delta}{3} J_{FV}(M, \Delta, L) + \frac{\Delta^2 - M^2}{3} K_{FV}(M, \Delta, L) \right], \quad (6.22)$$

with

$$K_{FV}(M, \Delta, L) \equiv \frac{\partial}{\partial \Delta} J_{FV}(M, \Delta, L), \quad (6.23)$$

and $\delta_1(ML)$ as given in Eq. (6.5).

Before turning to the fit details and results, we briefly discuss the extent to which including the splittings as in Eq. (6.20), and not other possible $1/M_H$ effects, is a systematic improvement on Eq. (6.2). In fact, in a parametric sense within the power counting introduced by Boyd and Grinstein [82], this is a systematic improvement, as long as we make some further specifications as to how Eq. (6.20) should be applied. As we detail below, however, the power counting of Ref. [82] is only marginally applicable to our data. For that reason we ultimately fit to both Eq. (6.20) and Eq. (6.2) and take the difference as one measure of the chiral extrapolation error.

For the following discussion, let Δ be a generic splitting (Δ^* or δ_{eq} or a linear combination of the two), and M be a generic light pseudoscalar mass. The power counting introduced in Ref. [82] takes

$$\frac{\Delta^2, \Delta M, M^2}{M_H} \ll \Delta \sim M. \quad (6.24)$$

For our data, treating Δ and M as the same size is not dangerous, even though Δ is significantly smaller than our simulation M values—at worst this means that we include some terms unnecessarily. The condition $M^2/M_H \ll \Delta$, which is necessary to drop other $1/M_H$ contributions as still higher order, is marginally valid, however. For the D system, $M_K^2/M_D \approx 130$ MeV, which is roughly of the same size as Δ^* and δ_{sd} . For the B system, $M_K^2/M_B \approx 47$ MeV, of the same size as Δ^* but somewhat less than δ_{sd} . For the purposes of the chiral extrapolation, however, what matters is the applicability of the power counting at the lowest simulated light meson masses, not its applicability at M_K .² For our lightest simulated pions with mass $\sim M_K/2$, we can reduce the left hand side of the inequality in Eq. (6.24) by a factor of four, at which point it becomes reasonably applicable.

Having tentatively accepted the power counting of Eq. (6.24), it is clear that $F(M/\Delta)$ in Eq. (6.17) should be treated as $\mathcal{O}(1)$. Then the difference between $J(M, \Delta)$ and the chiral logarithm it replaces, $\ell(M^2)$ is of the same order as $\ell(M^2)$ itself, so including the splittings becomes mandatory at the one-loop order to which we are working. The next question is whether Eq. (6.2) includes *all* effects to this order. As discussed by Boyd and Grinstein, the key issue is whether operators with two or more derivatives (two or more powers of residual momentum $\mathbf{k}$) on the heavy fields can contribute. Such operators are suppressed by $1/M_H$ relative to the leading-order heavy-light Lagrangian, which has a single derivative. Since we are keeping Δ^* , which is also in principle a $1/M_H$ effect, one might worry that such operators could contribute at the same order. The power counting implies, however, that the relevant diagrams pick up a factor of $(\Delta, M)/M_H$ relative to the terms being kept in

² We assume here that the fit to the data is good over the full mass range simulated. It is not important for the chiral extrapolation that the fit be systematic in the region around M_K , but it must describe the data in that range so that we can correctly interpolate to the physical kaon mass.

Eq. (6.20). The reason for the difference is that the explicit extra factor of $\mathbf{k}$ turns into Δ or M —the only dimensional constants available—after integration. In the term that generates the hyperfine splitting itself, in contrast, the dimensional quantity balanced against $1/M_H$ is Λ —a heavy-quark QCD scale—rather than M . The power counting in Eq. (6.24) effectively treats Λ as larger than M (so that $\Delta \sim \Lambda^2/M_H \sim M$). Similarly, the term that generates the flavor splittings has a single factor of m_q and no residual momentum, and Eq. (6.24) effectively takes $m_q \sim \mathbf{k}$ in such terms.

Boyd and Grinstein do find some other contributions at the same order as Eq. (6.20), but most come from terms that are simply Λ/M_H times terms in the leading-order heavy-light Lagrangian or current, and thus give simply an overall factor times the result without them. The exceptions are the terms multiplied by g_2 in Eq. (15) of Ref. [82] and by ρ_2 in Eq. (18) of Ref. [82]. These are operators that have the same dimension as the original Lagrangian current operators, but that violate heavy-quark spin symmetry, and therefore give different contributions to the pseudoscalar and vector meson decay constants at this order. Since we are only looking at pseudoscalar meson decay constants here, however, and since these effects are flavor-independent, we can also absorb all of the $1/M_H$ effects into (1) the effects of the splittings in the loop, described by Eq. (6.20), and (2) an overall factor in front of the full one-loop result.

The overall factor in Eq. (6.20) is $1/(16\pi^2 f^2)$. Since f is not fixed at one loop, one should in any case allow it to vary over a reasonable range, which we take to be f_π to f_K . We allow such variations even when we fit to the form without splittings, Eq. (6.2). The difference between using f_π and f_K corresponds to a 45% change in the size of the one-loop coefficient, but produces only a 1 to 3 MeV change in the decay constants.³ We therefore assume that any further $1/M_H$ uncertainty in $1/(16\pi^2 f^2)$ has negligible effects on our results.

Finally, there is a question of whether terms coming from taste violations contribute something new at the same order in which we include splittings. Since taste-violating terms in the Lagrangian can enter just like light-quark masses, this is a possibility in principle. Corresponding to the terms in the quark masses that generate flavor splittings of heavy-light mesons (*cf.* Eq. (45) of Ref. [39]), there are taste-violating terms given in Eq. (51) of that paper. Just as for the quark-mass terms, however, we are only interested here in contributions that change the heavy-light meson mass, not ones coupling the mesons to pion fields. When the pion fields are set to zero, all the terms in Eq. (51) of Ref. [39] just give a constant heavy-light meson mass term proportional to a^2 that contributes equally to the H and H^* masses of all valence flavors. Terms that produce a hyperfine splitting would have to also violate heavy quark spin symmetry, and hence be of order $a^2\Lambda/M_H$. Similarly, terms that produce flavor splitting would need to violate flavor symmetry, and hence be of order $a^2 m_q/\Lambda_\chi$. Both such contributions are higher order in our power-counting. Since there is no splitting, there is no contribution to the decay constants because the effect will vanish when we put the external B or D meson on mass shell.

In our chiral fits, we take the physical light-quark masses, as well as the parameters B_0 , $a^2\Delta_\xi$, δ'_A , and δ'_V , from the MILC Collaboration’s results of rSXPT fits to light pseudoscalars masses and decay constants [12, 85] on ensembles that include lattice spacing $a \approx 0.15$ fm through $a \approx 0.06$ fm. Table XII shows the values used. In general, we use older MILC determinations since newer versions, *e.g.*, those in Ref. [66], do not cover the full range of lattice spacings employed here (but are consistent where they overlap). The exceptions are

³ Most of the change in the size of the overall coefficient is compensated by a change in the LECs that come from the fit to our data.

TABLE XII. Inputs to our heavy-light chiral fits taken from the MILC Collaboration’s light-meson chiral fits [12, 85]. The physical bare-quark masses m_u , m_d , $\hat{m} \equiv (m_u + m_d)/2$, and m_s are determined by demanding that the charged pion and kaons take their physical masses after the removal of electromagnetic effects. Errors in the masses are due to statistics, chiral extrapolation systematics, scale determination, and (for m_d and m_u) the estimate of electromagnetic effects, respectively. “Continuum” values are found from chiral fits that have been extrapolated to the continuum, but masses are still in units of the “fine” ($a \approx 0.09$ fm) lattice spacing, and with the fine-lattice value of the mass renormalization. Values for $r_1^2 a^2 \delta'_A$ and $r_1^2 a^2 \delta'_V$ take into account newer MILC analyses [66] as noted in the text. The light-meson analysis determining these quantities assumes that they scale like the taste-violating splittings Δ_ξ and are larger by a factor of 1.68 on the 0.15 fm lattices than on the 0.12 fm lattices, and smaller by a factor 0.35 on the 0.09 fm lattices than on the 0.12 fm lattices. The statistical and systematic errors on $r_1 B_0$ and $r_1^2 a^2 \Delta_\xi$ are not given here; such errors have negligible effect on the heavy-light decay constants.

Quantity	Lattice spacing			
	$a \approx 0.15$ fm	$a \approx 0.12$ fm	$a \approx 0.09$ fm	“continuum”
$am_s \times 10^2$	4.29(1)(8)(6)	3.46(1)(10)(5)	2.53(0)(6)(4)	2.72(1)(7)(4)
$a\hat{m} \times 10^3$	1.55(0)(3)(2)	1.25(0)(4)(2)	0.927(2)(27)(13)	0.997(2)(32)(14)
$am_d \times 10^3$	2.20(0)(4)(3)(5)	1.78(0)(6)(3)(4)	1.31(0)(4)(2)(3)	1.40(0)(5)(2)(3)
$am_u \times 10^4$	8.96(2)(17)(13)(49)	7.31(2)(23)(10)(40)	5.47(1)(16)(8)(30)	5.90(1)(19)(9)(32)
$r_1 B_0$	6.43	6.23	6.38	6.29
$r_1^2 a^2 \Delta_A$	0.351	0.205	0.0706	0
$r_1^2 a^2 \Delta_T$	0.555	0.327	0.115	0
$r_1^2 a^2 \Delta_V$	0.721	0.439	0.152	0
$r_1^2 a^2 \Delta_I$	0.897	0.537	0.206	0
$r_1^2 a^2 \delta'_A$	—	−0.28(6)	—	0
$r_1^2 a^2 \delta'_V$	—	0.00(7)	—	0

the values of the taste-violating hairpin parameters $r_1^2 a^2 \delta'_A$ and $r_1^2 a^2 \delta'_V$. For them, the newer analysis including two-loop chiral logarithms gives larger systematic errors and a changed sign of the central value of $r_1^2 a^2 \delta'_V$, which has always been consistent with zero. For these parameters, we therefore use the wider ranges listed in Table XII, which encompasses both types of analyses. For comparison, the results of the analysis of Ref. [85] were $r_1^2 a^2 \delta'_A = -0.30(1)(4)$ and $r_1^2 a^2 \delta'_V = -0.05(2)(4)$.

In order to fit Eq. (6.20) to our lattice data, it is also necessary to input values for the hyperfine splitting Δ^* and for λ_1 in Eq. (6.16). For B mesons, we have [51]

$$\Delta^* = M_{B^*} - M_B \approx 45.8 \text{ MeV}, \quad (6.25)$$

$$\delta_{sd} = M_{B_s} - M_B \approx 87.0 \text{ MeV}, \quad (6.26)$$

$$\lambda_1 \approx 0.192 \text{ GeV}^{-1}, \quad (6.27)$$

where we use $M_E = M_S = 0.6858(40) \text{ GeV}$ [67] and $M_Q = M_{\pi^0} \approx 135.0 \text{ MeV}$ to obtain λ_1

from the experimental data. Similarly, for D mesons, we have

$$\Delta^* = M_{D_0^*} - M_{D_0} \approx 142.1 \text{ MeV}, \quad (6.28)$$

$$\delta_{sd} = M_{D_s} - M_{D_{\pm}} \approx 98.9 \text{ MeV}, \quad (6.29)$$

$$\lambda_1 \approx 0.219 \text{ GeV}^{-1}. \quad (6.30)$$

In the chiral fit, we input the relevant physical Δ^* and λ_1 from either Eqs. (6.25)–(6.27) or (6.28)–(6.30), and then use Eq. (6.16) with the actual m_e and m_q from each data point, and B_0 the slope for a given ensemble, from Table XII. We emphasize here that B_0 comes from a simple tree-level chiral fit of light meson masses to Eq. (6.1). This is adequate for our purposes, since the resulting meson masses are only used within the one-loop chiral logarithms.

We can now present the actual chiral fits and show how we extract results and systematic errors from them. Recall that we compute ϕ_{H_q} for many combinations of the valence and light sea-quark masses, and at three lattice spacings: $a \approx 0.15, 0.12$, and 0.09 fm. We fit all the decay constant data to the form given either by Eq. (6.20) or by Eq. (6.2). One-loop finite-volume effects are included through Eq. (6.21) or Eq. (6.4). There are four unconstrained free parameters in our fits: the LO parameter ϕ_H^0 , and the one-loop LECs L_{val} , L_{sea} , L_a [Eq. (6.12)]. The central fit fixes the chiral coupling f at f_π , but a range of couplings are considered in alternative fits, as described in more detail in Sec. VII. Similarly, the H - H^* - π coupling g_π , which is poorly constrained by our data, is taken in the range 0.51 ± 0.20 . This encompasses a range of phenomenological and lattice determinations [83, 86–91], as discussed in Ref. [53]. In the central fit, g_π is held fixed at 0.51, while it is varied in alternative fits described in Sec. VII. Although changing g_π is equivalent to changing f when splittings are omitted [*cf.* Eq. (6.2)], the effects are inequivalent when splittings are included [*cf.* Eq. (6.20)]. This is especially true of the finite-volume effects, for which the splittings have the potential to produce significant changes [79].

Some additional parameters constrained by Bayesian priors are also included in the chiral fits, as discussed above. The taste-violating hairpin parameters δ'_V and δ'_A are given by the ranges in Table XII. In addition, up to six heavy-quark and up to seven light-quark lattice-spacing dependent terms, are added for investigation of discretization effects. Except where otherwise noted, all twelve such terms are included in the fits plotted below: this gives errors that include true statistical errors plus our estimate of discretization effects from the heavy quarks and generic (taste non-violating) discretization errors from the light quarks. In addition, some or all of the (mildly) constrained NNLO LECs, $Q_1, \dots, Q_4$, are included. Again, unless otherwise noted, the fits below include all four such parameters; such fits tend to give larger (and hence more conservative) errors than fits that restrict the number of these parameters. In total, there are 23 fit parameters in the central fits: the 19 constrained parameters listed in this paragraph, and the 4 unconstrained parameters listed in the previous paragraph.

B. Chiral fits and extrapolations for the D system

Figure 3 shows our central chiral fit to $r_1^{3/2}\phi_{D^+}$ and $r_1^{3/2}\phi_{D_s}$. Data from ensembles at $a \approx 0.15$ fm, $a \approx 0.12$ fm and $a \approx 0.09$ fm are shown, but the $a \approx 0.15$ fm ensembles are not included in the fit. The points and covariance matrix are obtained from Analysis I

(Sec. IV B) of the two-point functions. For clarity, only the unitary (full QCD) points are shown for ϕ_D (and approximately unitary for ϕ_{D_s}), but the fit is to all the partially-quenched data on the $a \approx 0.12$ fm and $a \approx 0.09$ fm ensembles. The fit properly takes into account the covariance of the data; χ^2/dof and the p value (goodness of fit) are reasonable, as shown. The points in Fig. 3 are plotted as a function of mass m_x , where, for ϕ_{D+} , the light valence mass m_q and the light sea mass m_l are given by $m_q = m_l = m_x$. For ϕ_{D_s} , only $m_l = m_x$ varies, while m_q is held fixed at the value m_{s_v} near the physical strange mass m_s .⁴ In order to be able to compare ensembles at different lattice spacings, we have adjusted the bare quark masses by the ratio $Z_m/Z_m^{0.09\text{fm}}$, where Z_m is the (one-loop) mass renormalization constant [92], and $Z_m^{0.09\text{fm}}$ is its value on the $a \approx 0.09$ fm ensembles.

The continuum extrapolation is carried out by taking the fitted parameters and setting $a^2 = 0$ in all taste-violating terms (parameterized by Δ_ξ , δ'_A , δ'_V , and L_a), all heavy-quark discretization effects (parameterized by z_E , z_X , z_Y , z_B , z_3 , and z_2) and all generic light-quark discretization effects (parameterized by C_i). The red lines (solid for ϕ_{D+} , dotted for ϕ_{D_s})

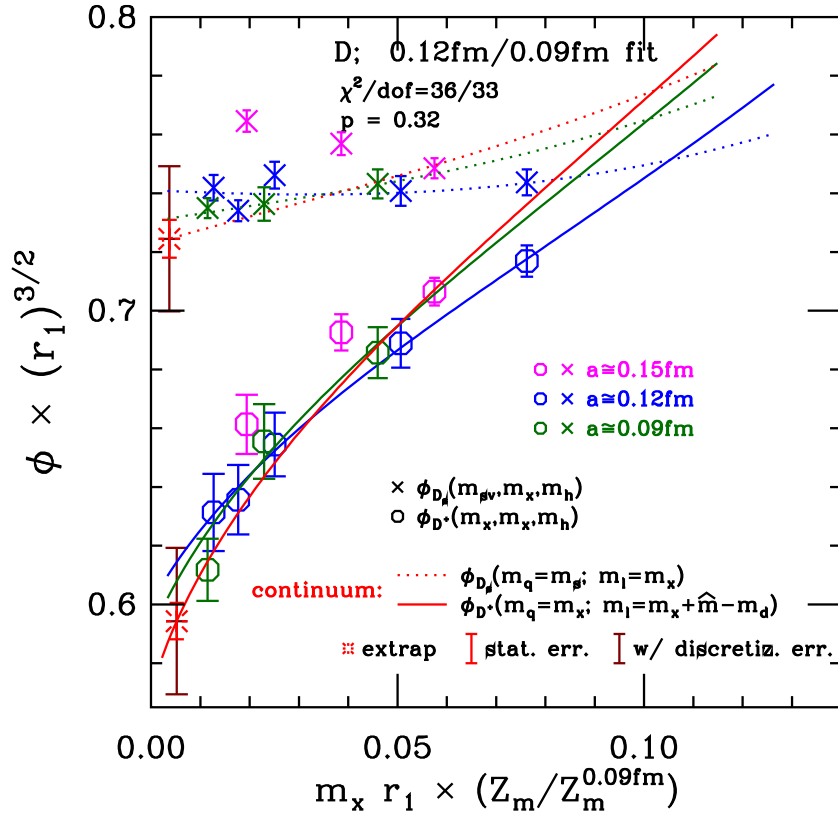


FIG. 3. Central chiral fit for the D system, based on Analysis I of the fits to 2-point correlators. Only (approximately) unitary points are shown. Data from ensembles at $a \approx 0.15$ fm, $a \approx 0.12$ fm and $a \approx 0.09$ fm are shown, but the $a \approx 0.15$ fm ensembles are not included in the fit. The bursts show extrapolated values for ϕ_{D_s} and ϕ_{D+} , with the purely statistical errors in bright red and the statistical plus discretization errors in darker red. The physical strange-quark mass corresponds to an abscissa value of $m_x \approx 0.1$.

⁴ On the $a \approx 0.15$ fm ensembles, m_{s_v} is equal to the value of the strange sea quark mass m_h ($am_{s_v} = 0.0484$), but on the other two ensembles we take it lower than m_h , because m_h has been chosen somewhat larger than the physical strange mass. In the figure, $am_{s_v} = 0.415$ for the $a \approx 0.12$ fm ensembles and $am_{s_v} = 0.272$ for the $a \approx 0.09$ fm ensembles.

show the effect of extrapolating to the continuum and setting the strange quark mass (both sea, m_h , and valence, m_{s_v}) to the physical value m_s .

Finally, the bursts give the result after the chiral extrapolation in the continuum, *i.e.*, setting $m_x = m_d$ for ϕ_{D^+} , and $m_x = \hat{m}$ for ϕ_{D_s} . The larger, dark red, error bars on the bursts show the total error from the fit, which includes heavy-quark and generic light-quark discretization errors using Bayesian priors, as described above. The smaller, bright red error bars, show purely statistical errors, which are computed by a fit with all the discretization prior functions turned off. In plotting the red line for ϕ_{D^+} , the light sea mass is shifted slightly ($m_l = m_x + \hat{m} - m_d$) so that it takes its proper mass when $m_x = m_d$. (We neglect isospin violations in the sea.) The small mass differences between $\hat{m}$ and m_d (and the corresponding difference between $\hat{m}$ and m_u for the B^+) produce changes in ϕ that are much smaller than our current errors, but we include them here with an eye to future work, where the precision will improve.

The trend of the data for the coarsest lattice spacing ($a \approx 0.15$ fm, the magenta points in Fig. 3) tends to be rather different than for the finer lattice spacings, especially for the D_s , which is why we exclude the $a \approx 0.15$ fm data from the central fit. This trend is even more exaggerated for the B system, but with particularly large statistical errors; see Fig. 6 below. Nevertheless, the effect of including the $a \approx 0.15$ fm points in the fit is a rough indication of the size of discretization errors. Figure 4 shows what happens to the fit when these points are included: ϕ_{D^+} and ϕ_{D_s} each move up an amount comparable to (but less than) the size of the larger (dark red) error bars, which represent heavy and generic light quark discretization errors (as well as statistical errors, which are smaller). The consistency is reassuring.

As discussed in Sec. IV, we also examine Analysis II of the 2-point functions. Figure 5 shows the effect of using Analysis II in the chiral fits. The differences in the decay constant results between Fig. 3 and Fig. 5 are included in the decay-constant error budgets as a “fitting error”. Note that the covariance matrix calculation in Analysis II results in an apparent underestimate of χ^2 (and, consequently, a high apparent p value). We believe that this stems from binning of the data to remove autocorrelation effects, which has the disadvantage of reducing the number of samples used to compute the covariance matrix. It is then difficult to determine small eigenvalues accurately. Indeed the eigenvalues of the (normalized) correlation matrix tend to have a lower bound of $\sim 10^{-4}$ to 10^{-3} with this approach, whereas they typically go down to 10^{-5} in Analysis I. [Recall that in Analysis I we keep all samples, and deal with autocorrelation effects by Eq. (4.13).] Nevertheless, the difficulty with small eigenvalues explains only a small fraction of the difference between the results from Analyses I and II. For example, f_D is changed by only 0.2 MeV when we smooth eigenvalues from Analysis I that are less than 10^{-3} , following the method of Ref. [93]. This may be compared to the total difference between f_D in Analyses I and II, which is 1.7 MeV.

C. Chiral fits and extrapolations for the B system

Results for the B system closely resemble those for the D system in most respects. One important difference is that the signal-to-noise ratio is worse for the B system because the mass difference that controls the noise, $2m_B - m_{\eta_b} - m_\pi$, increases with the mass of the heavy quark [94]. Therefore, the preferred fit in Analysis I for the charm case (1 simple exponential + 1 oscillating exponential at large t_{min}) is too noisy here, and we must use fits with an extra excited state and smaller t_{min} (see Sec. IV B). Consequently, our B -system

results have larger statistical errors. On the other hand, heavy-quark discretization errors are smaller in the B system. In the HQET analysis of discretization effects they appear in the heavy-quark expansion, which works better for B 's to begin with [60].

Figure 6 shows, for unitary points only, our central chiral fit for the B system. This is based on Analysis I of the 2-point functions. As in Fig. 3, the red lines (solid for ϕ_{B^+} , dotted for ϕ_{B_s}) show the effect of extrapolation to the continuum and setting the strange quark mass to its physical value m_s . For the solid red line, the light sea mass is again shifted slightly, but now $m_l = m_x + \hat{m} - m_u$, so that it takes its proper mass when $m_x = m_u$. The bursts show the final results, and come from setting $m_x = m_u$ for ϕ_{B^+} and $m_x = \hat{m}$ for ϕ_{B_s} . As before, the smaller, bright red, error bars, show purely statistical errors, and the larger, dark red, error bars come from the fit with Bayesian priors and include heavy-quark and generic light-quark discretization errors as well as statistical errors.

In Fig. 6, the $a \approx 0.15$ fm data are both noisy and far from those of the finer lattice spacings. Therefore, these ensembles are again dropped from the central fit. Figure 7 shows the effect of including the $a \approx 0.15$ fm points. Note that the resulting continuum-extrapolated line for ϕ_{B_s} (dotted red line) now has what appears to be a rather unphysical shape, showing a significant initial increase as the light sea-quark mass is decreased, starting at the right side of the graph. Hence, the differences caused by including the $a \approx 0.15$ fm points is 10 to 20% larger than the dark red error bars in Fig. 6, and 40 to 60% larger than discretization errors estimated by removing the statistical errors from the dark red bars. Because the trend for $a \approx 0.15$ fm is so different from the other spacings, and because of the unphysical behavior when these points are included in the fit, we believe this difference

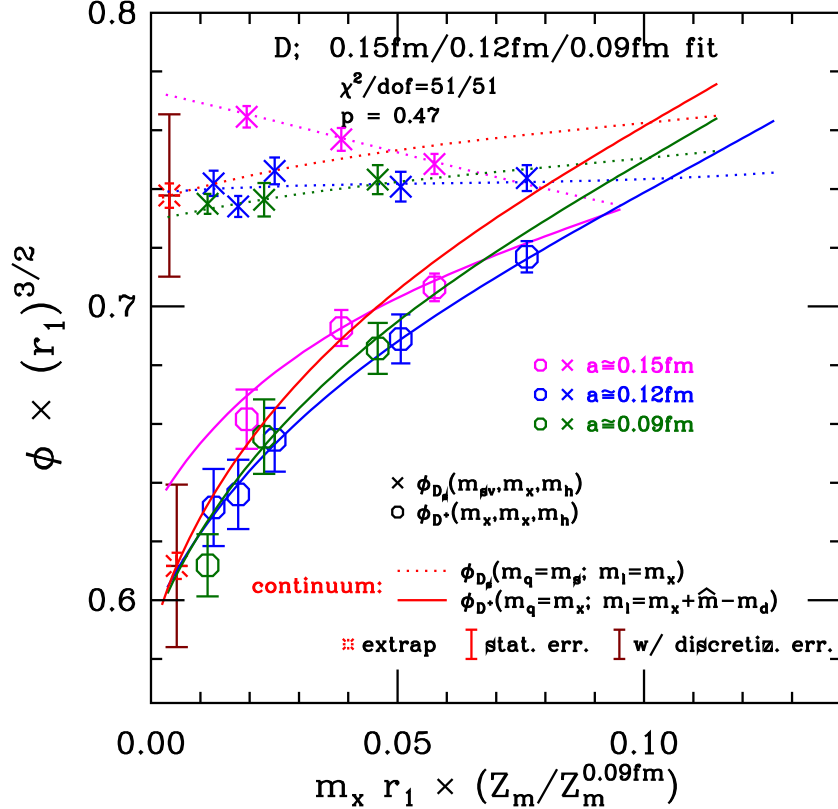


FIG. 4. Same as Fig. 3, but including points at $a \approx 0.15$ fm in the chiral-continuum fit.

overestimates the true discretization error, and we do not enlarge the errors coming from the fit.

Figure 8 shows the effect of using Analysis II of the correlation functions. In order to make these comparisons as direct as possible, we first turn off all the Bayesian discretization terms in the fits. Compared to the results from Fig. 6, this fit gives a value of f_{B_s} about 1 MeV higher and a value of f_{B^+} about 2 MeV lower. These differences are included in our estimate of the fitting errors due to excited state contamination in Sec. VII.

VII. ESTIMATION OF SYSTEMATIC ERRORS

In this section, we present a careful, quantitative accounting for the uncertainties in our calculation. We consider in turn discretization errors, fitting errors, errors from inputs r_1 and quark-mass tuning, renormalization, and finite-volume effects. Table XIII details our error budget.

A. Heavy-quark and generic light-quark discretization effects

As described in Sec. VI and Appendix A, we parameterize possible heavy-quark and generic light-quark discretization effects and follow a Bayesian approach in including such effects in our chiral fitting function. Consequently, the raw “statistical” error that comes from our fits is not a pure statistical error but includes an estimate of the errors coming

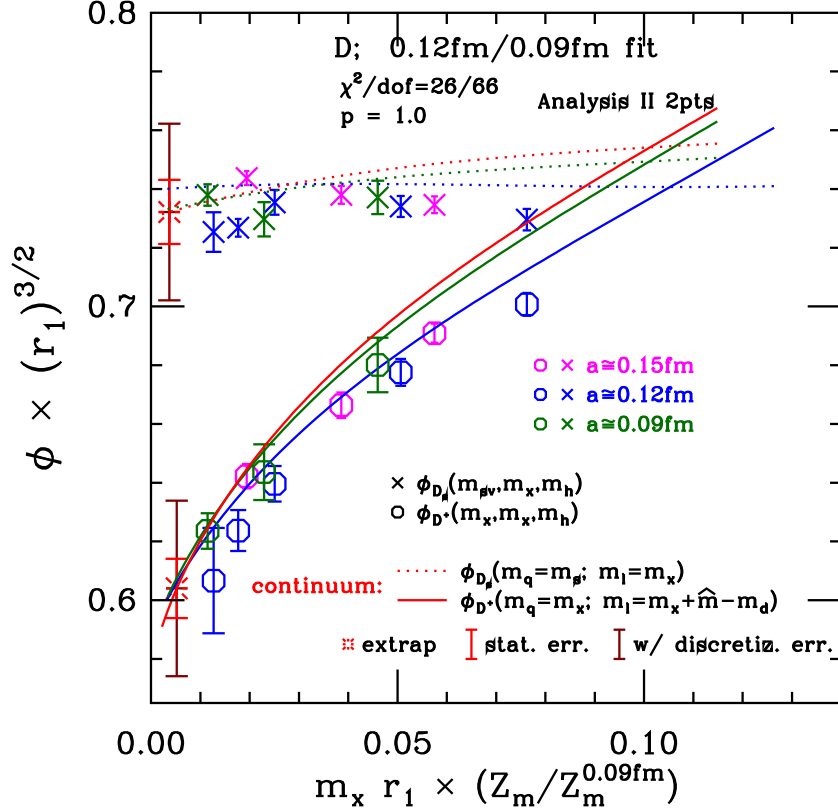


FIG. 5. Same as Fig. 3, but using Analysis II of the 2-point function.

from the discretization effects. This inclusive error is shown with the dark red error bars in the plots in Sec. VI, and is listed in the first line of Table XIII.

For informational purposes, it is useful to break down this inclusive error into its component parts, at least approximately. We can see what errors to expect and, hence, target for improvement in future simulations. In particular, with our current actions, the light-quark and heavy-quark discretization errors should behave differently as a function of lattice spacing, with heavy-quark errors decreasing more slowly as a is reduced. To extract the pure statistical errors, we rerun the fits with all the Bayesian discretization terms set to zero. We then find the pure heavy-quark (or pure light-quark) discretization contributions, by turning back on the heavy-quark (light-quark) terms, and then subtracting in quadrature the pure statistical errors from the resulting raw errors. These individual errors are shown in Table XIII in parentheses. Note that the total error at the bottom of the table includes the error on the first line, not the sum of the three errors in parentheses, when these differ. Note also that the discretization errors are similar to what we would have obtained with less sophisticated power counting.

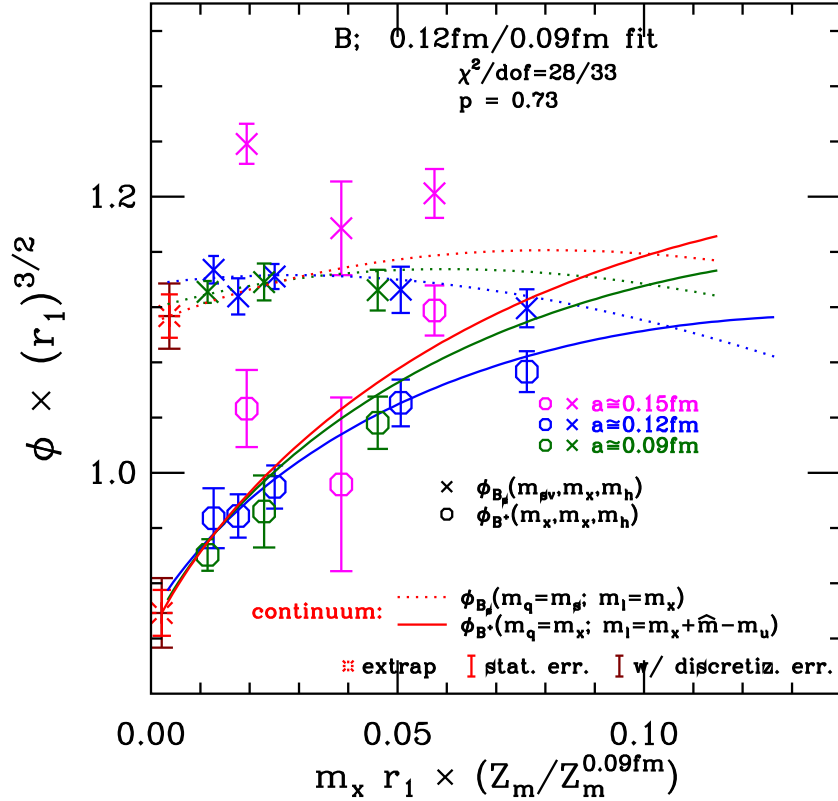


FIG. 6. Central chiral fit for the B system, with data from Analysis I of the 2-point functions. Only (approximately) unitary points are shown. Data from ensembles at $a \approx 0.15$ fm, $a \approx 0.12$ fm, and $a \approx 0.09$ fm are shown, but the $a \approx 0.15$ fm ensembles are not included in the fit. The bursts show extrapolated values for ϕ_{B_s} and ϕ_{B^+} , with the purely statistical errors in bright red and the statistical plus discretization errors in darker red. The physical strange-quark mass corresponds to an abscissa value of $m_x \approx 0.1$.

B. Chiral extrapolation and taste-violating light-quark discretization effects

As described in Sec. VI, we modify the chiral fit function in a variety of ways to estimate the error associated with the chiral extrapolation:

- $\chi 1$. Set the chiral coupling f to f_K instead of f_π .
- $\chi 2$. Allow the chiral coupling f to be a Bayesian fit parameter, with prior value f_π and prior width equal to $f_K - f_\pi$.
- $\chi 3$. Replace the H - H^* - π coupling g_π (which is 0.51 in the central fit) with 0.31 or 0.71, which are the extremes of the range discussed in Sec. VI.
- $\chi 4$. Allow g_π to be a constrained fit parameter, with prior value 0.51 and prior width 0.20.
- $\chi 5$. Fix to zero those NNLO analytic terms [Q_2 and/or Q_4 in Eq. (6.15)] that may be eliminated without making the fit unacceptably poor.
- $\chi 6$. Use the chiral function without hyperfine and flavor splittings, *i.e.*, use Eq. (6.2) instead of Eq. (6.20).
- $\chi 7$. Use combinations of modifications $\chi 1$ and $\chi 3$ or modifications $\chi 2$ and $\chi 3$. These choices can produce significantly larger deviations since changes in g_π have a similar effect on the fit function as changes in f .

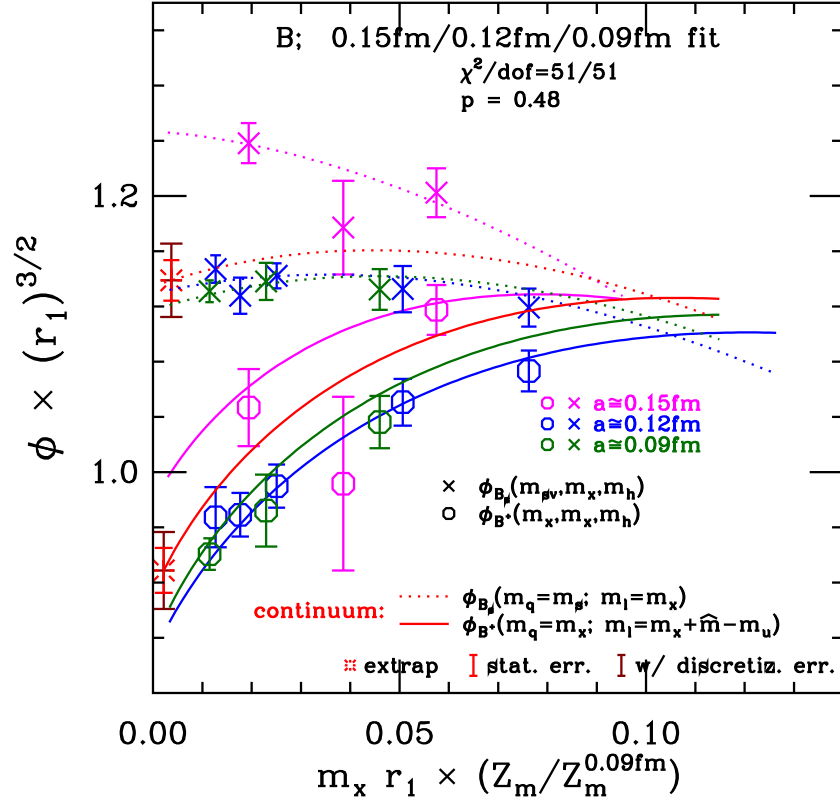


FIG. 7. Same as Fig. 6, but including points at $a \approx 0.15$ fm in the fit.

TABLE XIII. Total error budget for the heavy-light decay constants. Uncertainties are in MeV for decay constants. The total combines errors in quadrature. The first row includes statistics, heavy-quark discretization errors, and generic light-quark discretization errors, as explained in the text. Errors in parentheses are approximate sub-parts of errors that are computed in combination.

Source	f_{D^+} (MeV)	f_{D_s} (MeV)	f_{D_s}/f_{D^+}	f_{B^+} (MeV)	f_{B_s} (MeV)	f_{B_s}/f_{B^+}
Statistics $\oplus$ discretization	9.2	8.9	0.014	5.5	5.1	0.013
(statistics)	(2.3)	(2.3)	(0.005)	(3.6)	(3.4)	(0.010)
(heavy-quark disc.)	(8.2)	(8.3)	(0.007)	(3.7)	(3.8)	(0.004)
(light-quark disc.)	(2.9)	(1.5)	(0.012)	(2.5)	(2.1)	(0.007)
Chiral extrapolation	3.2	2.2	0.014	2.9	2.8	0.014
Two-point functions	3.3	1.6	0.013	3.0	4.1	0.015
Scale (r_1)	1.0	1.0	0.001	1.0	1.4	0.001
Light quark masses	0.3	1.4	0.005	0.1	1.3	0.006
Heavy quark tuning	2.8	2.8	0.003	3.9	3.9	0.005
u_0 adjustment	1.8	2.0	0.001	2.5	2.8	0.001
Finite volume	0.6	0.0	0.003	0.5	0.1	0.003
$Z_{V_{Q\bar{Q}}}^4$ and $Z_{V_{q\bar{q}}}^4$	2.8	3.4	0.000	2.6	3.1	0.000
Higher-order $\rho_{A_4}^{Qq}$	1.5	1.8	0.001	1.4	1.7	0.001
Total Error	11.3	10.8	0.025	8.9	9.5	0.026

The central fits give

$$L_a = +0.6 \pm 6.5 \quad (D \text{ system}), \quad (7.1)$$

$$L_a = -1.9 \pm 8.8 \quad (B \text{ system}), \quad (7.2)$$

where the error is the raw statistical error. (Note that we do not constrain L_a by any prior width.) The errors in L_a decrease by about 10% if Bayesian parameters for generic light-quark errors are removed, and an additional 10% if the parameters for heavy-quark errors are removed. Thus, there is “cross talk” between various error sources, making it difficult to completely distinguish the various types of discretization errors. Future work, with more and finer lattice spacings, should make a cleaner separation possible.

C. Fitting errors

The “fitting errors” are the errors introduced in the analysis of the two-point correlators. They represent the effects of various choices of fit ranges and fitting functions, and are an estimate of the systematic effect of the contamination by excited states. We compare results from the three choices of two-point fitting (see Sec. IV): Analysis I, Analysis II, and a modified Analysis I using 1 simple + 1 oscillating state, but values of t_{min} larger than those described in Sec. IV B.

Some of these differences may, in fact, be due simply to statistical effects, and hence already included in the statistical error. Figure 11 shows the differences between values of ϕ_{B_q} in Analyses I and II, divided by the average statistical error for each of the common partially quenched data points. Only 10 of 74 differences are greater than 1 statistical σ .

Nevertheless, there appears to be some significant systematic trend in that 46 of 74 points are positive. To be conservative, we take the largest difference between the Analysis-I fits and the other two fits as the fitting error for each physical quantity, and list it in Table XIII. For f_{D_s} and f_{B_s} , the difference is largest for chiral fits based on 2-point Analysis II, while, for the other four quantities, the difference is largest for the modified Analysis I.

D. Scale uncertainty

We use the scale $r_1 = 0.3117(22)$ fm to tune the values of the quark masses and convert the decay constants into physical units (see Sec. III A). To find the scale errors on the final results, we shift r_1 to 0.3139 fm or 0.3095 fm and redo the analysis. Although ϕ_H scales like $r_1^{-3/2}$, the change in the results under a change in r_1 is smaller than pure dimensional analysis would imply, because our estimates of the physical light masses and the heavy-quark κ_c and κ_b also shift, producing partially compensating changes in ϕ_H . At $r_1 = 0.3139$ fm, we shift the light masses in Table XII upward by the scale error shown in that table. [The lattice light-quark masses scale like r_1^2 , because they are approximately linear in the squared meson masses $(r_1 m_\pi)^2$ and $(r_1 m_K)^2$.] Similarly, we shift the tuned κ_c and κ_b downward by the scale error in Table V because the bare heavy quark mass increases with r_1 . We then adjust $\phi_{B(s)}$ and $\phi_{D(s)}$ at each lattice spacing using Eq. (3.5) and the values of $d\phi/d\kappa$ given in Table V. Redoing the preferred chiral fits shown in Figs. 3 and 6, extrapolating to the

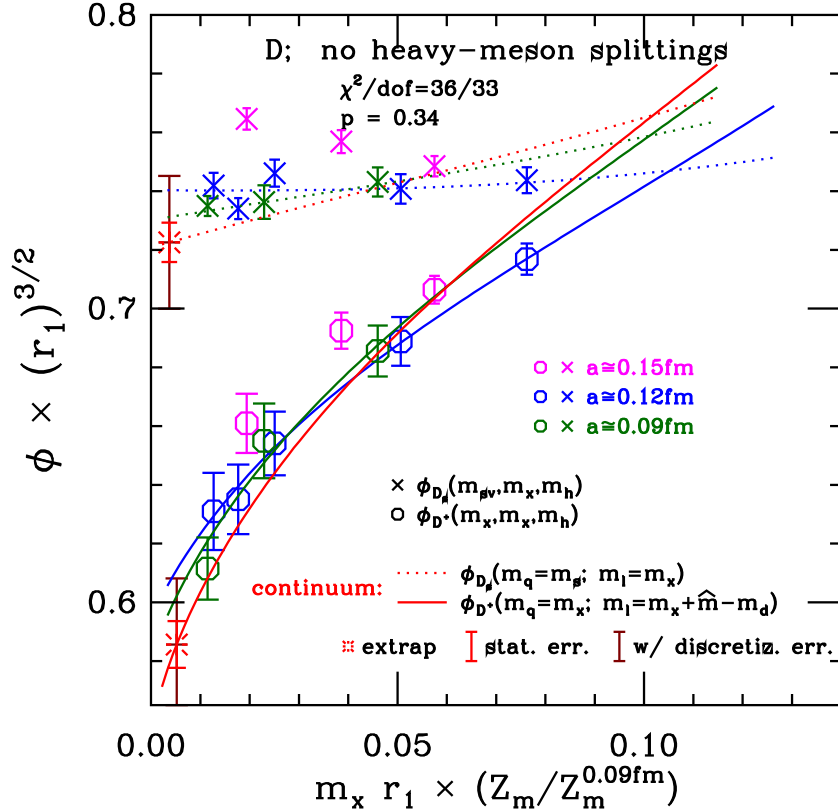


FIG. 9. Same as Fig. 3 but omitting heavy-light hyperfine and flavor splittings in the chiral fit function.

continuum, and plugging in the adjusted continuum light quark masses gives the scale error listed in Table XIII.

E. Light-quark mass determinations

To estimate the error from the light-quark mass determination, we follow a similar procedure to that in the scale-error case. We shift the continuum light quark masses in Table XII by the sum in quadrature of all errors except scale errors. This includes the statistical errors, the chiral errors and, where relevant, the electromagnetic errors. We then plug the new masses into the continuum-extrapolated chiral fits and take the difference from the central results to give the errors listed in Table XIII. The relative direction of shifts on different masses makes little difference in the size of the errors on the decay constants f_{D_s} , f_{D^+} , f_{B_s} , and f_{B^+} , since they are sensitive primarily to the valence quark masses. However, it does affect the error of the ratios f_{D_s}/f_{D^+} and f_{B_s}/f_{B^+} . The largest effect clearly occurs when the strange mass is shifted in the opposite direction from the lighter masses. To be conservative, we take the size of change of the ratios in this case as the error, but this is almost certainly an overestimate because the statistical and chiral extrapolation errors on the light quark masses are positively correlated between the strange mass and the other masses.

Note that the errors from the light-quark masses in Table XIII are much larger for f_{D_s} and f_{B_s} than for f_{D^+} and f_{B^+} . That simply reflects the facts that the decay constants have a nonzero limit when the quark masses vanish, and that the dependence on the quark masses is reasonably linear. Thus a given percent error in the strange mass produces a much larger

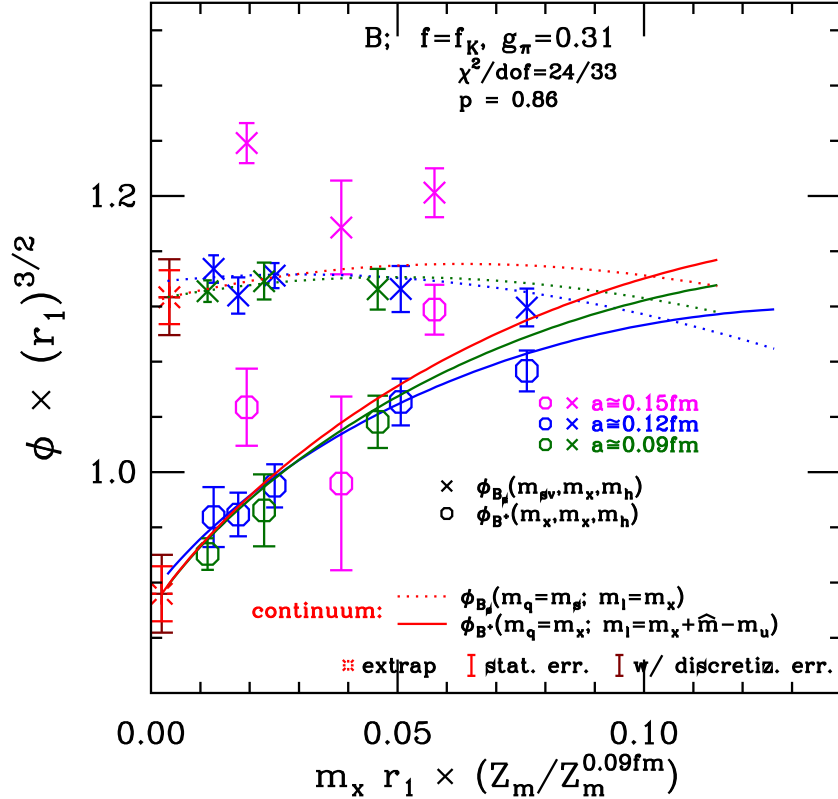


FIG. 10. Same as Fig. 6 but with $f = f_K$ and $g_\pi = 0.31$ in the chiral fit function.

percent difference in f_{D_s} and f_{B_s} , than the same percent error in the d or u mass does in f_{D^+} and f_{B^+} .

F. Bottom and charm quark mass determinations

The propagation of statistical errors in the tuned κ_c and κ_b to the decay constants is complicated by the fact that the independent errors at each lattice spacing affect the final results in a nontrivial way through the continuum and chiral extrapolations. At each lattice spacing, we choose 200 gaussian-distributed ensembles of trial κ values with central value equal to the tuned values, and standard deviation equal to the statistical error, taken from Table V. For a given choice of trial κ values at each lattice spacing, we produce an adjusted trial data sample by shifting the ϕ_H values according to Eq. (3.5), but with the trial values replacing the tuned values. We then perform the complete chiral fit and extrapolation

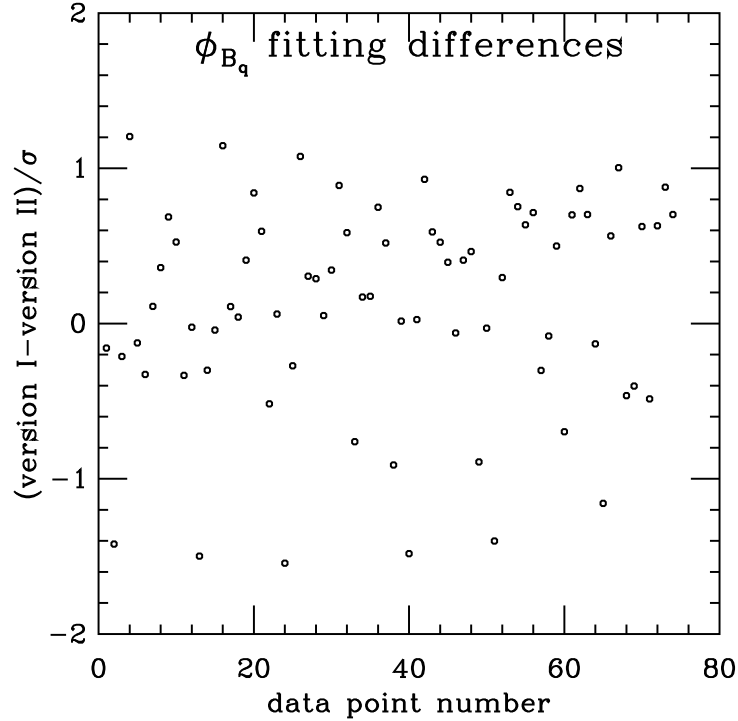


FIG. 11. Difference of ϕ_{B_q} values from Analyses I and II, divided by the average statistical error at each of the common valence and sea mass points. The order along the abscissa is arbitrary.

procedure on each of the 200 trial data sets. The standard deviation over trials of a given decay constant or decay constant ratio is taken to be the heavy quark tuning error, and is listed in Table XIII.

G. Tadpole factor (u_0) adjustment

In order to improve the convergence of lattice perturbation theory, we use tadpole-improved actions for the gluons, light quarks, and heavy quarks [76]. For the gluon and sea-quark actions we take the tadpole factor u_0 from the average plaquette. On the $a \approx 0.15$ fm and $a \approx 0.09$ fm lattices we use the same choice for the light valence and heavy-quark actions. On the $a \approx 0.12$ fm lattices, however, we use the tadpole factor u_0 taken from the Landau link in the valence-quark action and in the clover term in the heavy-quark action. This results in a slight mismatch between the light valence and sea-quark actions on these ensembles, and also affects the values obtained for the tuned bottom- and charm-quark masses κ_b and κ_c . The difference between u_0 obtained from the average plaquette and the Landau link is approximately 3–4% on the $a \approx 0.12$ fm ensembles.

We propagate this difference through the chiral/continuum extrapolation as follows. First, we compute the heavy-strange meson decay amplitudes ϕ_{B_s} and ϕ_{D_s} with both choices for u_0 on the ensemble with $am_l/am_h = 0.01/0.05$, $a \approx 0.12$ fm. For each choice of u_0 , we compute ϕ_{B_s} and ϕ_{D_s} directly at the tuned values of κ_b and κ_c , thereby avoiding an interpolation in κ . Next, we renormalize the lattice decay amplitudes using the nonperturbative, flavor-diagonal current renormalization factors $Z_{V_{qq}^4}$ and $Z_{V_{Qq}^4}$ obtained for each case. (We neglect the slight difference in the perturbative correction $\rho_{A_{Qq}^4}$.) Then, we calculate the ratio of the renormalized decay amplitudes, finding no difference within errors:

$$\phi_c^{\text{plaquette}}/\phi_c^{\text{Landau}} = 1.005(13), \quad (7.3)$$

$$\phi_b^{\text{plaquette}}/\phi_b^{\text{Landau}} = 1.014(20). \quad (7.4)$$

As expected, the u_0 dependence from the bare current and renormalization factors mostly cancels. Finally, we repeat the chiral/continuum extrapolation shifting ϕ_c and ϕ_b on the $a \approx 0.12$ fm ensembles by the statistical errors reported in Eqs. (7.3)–(7.4). We find that these percent-level errors in ϕ_c and ϕ_b lead to approximately 1% errors in the extrapolated decay constants and approximately 0.1% errors in the decay-constant ratios. These errors are listed as “ u_0 adjustment” in the error budget in Table XIII.

H. Heavy-light current renormalization

There are two sources of systematic error in our heavy-light current renormalization. The first is due to the perturbative calculation of $\rho_{A_{Qq}^4}$ and the second is due to the nonperturbative calculation of $Z_{V_{qq}^4}$ and $Z_{V_{Qq}^4}$.

The perturbative calculation of $\rho_{A_{Qq}^4}$ has been carried out to one-loop order. Since $\rho_{A_{Qq}^4}$ is defined from a ratio of renormalization factors [see Eq. (2.5)], its perturbative corrections are small by construction. Indeed, as can be seen from the results for $\rho_{A_{Qq}^4}$ given in Table VIII, we observe very small corrections. For bottom they range from 0.3% at $a \approx 0.09$ fm to 0.8% at $a \approx 0.12$ fm and 2.8% at $a \approx 0.15$ fm. For charm they range from less than 0.08% at $a \approx 0.09$ fm to 0.4% at $a \approx 0.12$ fm and 0.6% at $a \approx 0.15$ fm. As shown in Ref. [43] the

perturbative corrections to the ρ -factors for the spatial currents, while still small, tend to be bigger than those for the temporal currents A^4 and V^4 . We therefore estimate the error due to neglecting higher order terms as $\rho_{V_{Qq}^1}^{[1]} \alpha_s^2$. We take α_s at $a \approx 0.09$ fm and $\rho_{V_{Qq}^1}^{[1]} \approx 0.1$, which is the largest one-loop coefficient for $\rho_{V_{Qq}^1}$ in the mass range $m_Q a \leq 3$. This procedure yields a systematic error of 0.7%, which we take for both charm and bottom decay constants.

The decay constant ratios f_{B_s}/f_{B^+} and f_{D_s}/f_{D^+} depend on the corresponding ratios of $\rho_{A_{Qq}^4}/\rho_{A_{Qq}^4}$. These ratios differ from unity only because of the small variation of the $\rho_{A_{Qq}^4}$ with light valence mass, which is described in Sec. V. We take the variation of the $\rho_{A_{Qq}^4}$ with light valence mass at $a \approx 0.09$ fm as the error. This yields an error of 0.1% for both bottom and charm.

The dominant corrections in the heavy-light renormalization factor as defined in Eq. (2.5) are due to $Z_{V_{Qq}^4}$ and $Z_{V_{QQ}^4}$ which are calculated nonperturbatively. The values (and errors) for $Z_{V_{q\bar{q}}^4}$ and $Z_{V_{Q\bar{Q}}^4}$ are listed in Tables IX and XI, respectively. To obtain the error in $Z_{V_{Qq}^4} = \sqrt{Z_{V_{q\bar{q}}^4} Z_{V_{Q\bar{Q}}^4}}$ we add the statistical errors in $Z_{V_{q\bar{q}}^4}$ and $Z_{V_{Q\bar{Q}}^4}$ in quadrature. The error on $Z_{V_{Qq}^4}$ is dominated by the error on $Z_{V_{q\bar{q}}^4}$. The errors are largest, 1.3%, on the $a \approx 0.09$ fm ensemble and they are about the same for both charm and bottom on the two finest ensembles used to obtain our main decay constant results. Hence we use 1.3% as our estimate for the uncertainty in $Z_{V_{Qq}^4}$.

I. Finite volume effects

To study finite volume effects, we use the chiral fit function with heavy-light hyperfine and flavor splittings included (Eq. (6.20)), since the effects are known to be larger with the splittings than without [79]. The central fit includes the (one-loop) finite volume corrections, Eq. (6.21), on the lattice data, and then takes the infinite volume limit when extracting the final results for the decay constants. We then take the larger of the following two values as our estimate of the finite volume error:

- V1. The difference between the central result and the result from a chiral fit in which the finite volume corrections are omitted.
- V2. The largest finite volume correction to the relevant data points, as determined by the central fit. For ϕ_{D^+} and ϕ_{B^+} , the “relevant data points” are the ones on each ensemble with the lightest valence mass, *i.e.*, those closest to the chirally extrapolated point. For ϕ_{D_s} and ϕ_{B_s} , the relevant points are the ones on each ensemble with valence mass closest to m_s .

Method V1 gives a larger difference for ϕ_{D_s} and ϕ_{B_s} ; method V2 for ϕ_{D^+} and ϕ_{B^+} and the ratios. The resulting values are shown in Table XIII. Note that our choices are conservative because we correct for the (one-loop) finite volume errors, but nevertheless take the full size of these effects as our error.

VIII. RESULTS AND CONCLUSIONS

After adding the error estimates described in the previous section in quadrature, we obtain:

$$f_{B^+} = 196.9(8.9) \text{ MeV}, \quad (8.1)$$

$$f_{B_s} = 242.0(9.5) \text{ MeV}, \quad (8.2)$$

$$f_{B_s}/f_{B^+} = 1.229(0.026), \quad (8.3)$$

$$f_{D^+} = 218.9(11.3) \text{ MeV}, \quad (8.4)$$

$$f_{D_s} = 260.1(10.8) \text{ MeV}, \quad (8.5)$$

$$f_{D_s}/f_{D^+} = 1.188(0.025). \quad (8.6)$$

Since our most reliable method of determining discretization errors combines them with statistical errors, we do not quote separate statistical and systematic errors.

Figure 12 shows a comparison of our results for charmed decay constants with other lattice QCD calculations and with experiment. Our results agree with the only other three-flavor lattice QCD determination from the HPQCD collaboration [95], which is obtained with HISQ staggered valence quarks and asqtad staggered sea quarks. (The difference in f_{D_s} is a bit greater than 1σ .) They are also consistent with the two-flavor results of the ETM Collaboration using twisted-mass Wilson fermions [96], although the ETM error budget does not include an estimate of the uncertainty due to quenching the strange quark. One can also compare with “experimental” determinations of f_D and f_{D_s} if one assumes CKM unitarity to obtain the matrix elements $|V_{cd}|$ and $|V_{cs}|$. For the D meson, Rosner and Stone combine CLEO’s measurement of branching fraction $\mathcal{B}(D^+ \rightarrow \mu^+\nu)$ [97] with the latest determination of $|V_{cd}|$ from the PDG [51] to obtain $f_D = 206.7(8.9) \text{ MeV}$ [50]. For the D_s meson, they average CLEO and Belle results for $\mathcal{B}(D_s^+ \rightarrow \mu^+\nu)$ [98, 99] with CLEO and BABAR results for $\mathcal{B}(D_s^+ \rightarrow \tau^+\nu)$ [98, 100–102] to obtain a combined average for the two decay channels of $f_{D_s} = 257.5(6.1) \text{ MeV}$ [50]. The Heavy Flavor Averaging Group obtains a similar average, $f_{D_s} = 257.3(5.3) \text{ MeV}$ [103]. Our results are consistent with these values, confirming Standard Model expectations at the $\sim 5\%$ level.

Figure 13 shows a similar comparison of our results for bottom meson decay constants with other lattice QCD calculations. Our results agree with the published three-flavor determination using NRQCD b -quarks and Asqtad staggered light quarks of the HPQCD collaboration [105], but are only marginally consistent with HPQCD’s more recent calculation of f_{B_s} using HISQ light valence quarks [104]. Our results are also consistent with the two-flavor results of the ETM collaboration [96], who use Wilson heavy quarks and interpolate between the charm-mass region and the static limit to obtain results for bottom. Further, our result for the ratio f_{B_s}/f_B also agrees with the significantly less precise three-flavor determination using static b -quarks and domain-wall light quarks by the RBC and UKQCD Collaborations [106].

For the D system the largest uncertainties in our current calculation stem from heavy-quark discretization, while the chiral extrapolation, the Z_V factors, excited states, heavy-quark tuning, and the chiral-continuum extrapolation play important but subdominant roles. For the B system, heavy-quark tuning, statistics, and excited states are the sources of the largest errors, while the Z_V factors and the chiral-continuum extrapolation (incorporating our estimate of heavy-quark discretization effects) are next in size. Recall that a novel feature of our work is the treatment of heavy-quark discretization effects, via the functions

f_i in Eq. (2.4), and priors constraining the chiral-continuum fits to follow this form. At tree level, we have explicit calculations of the mismatch, some of which appeared already in Ref. [33] and all of which are compiled in Ref. [60]. Beyond the tree level, the continuum and static limits can be used to constrain the functional form. That said, the theoretical guidance of the priors cannot be highly effective in an analysis, such as this, with only two lattice spacings. Indeed, the quoted heavy-quark discretization errors are similar to less sophisticated power-counting estimates.

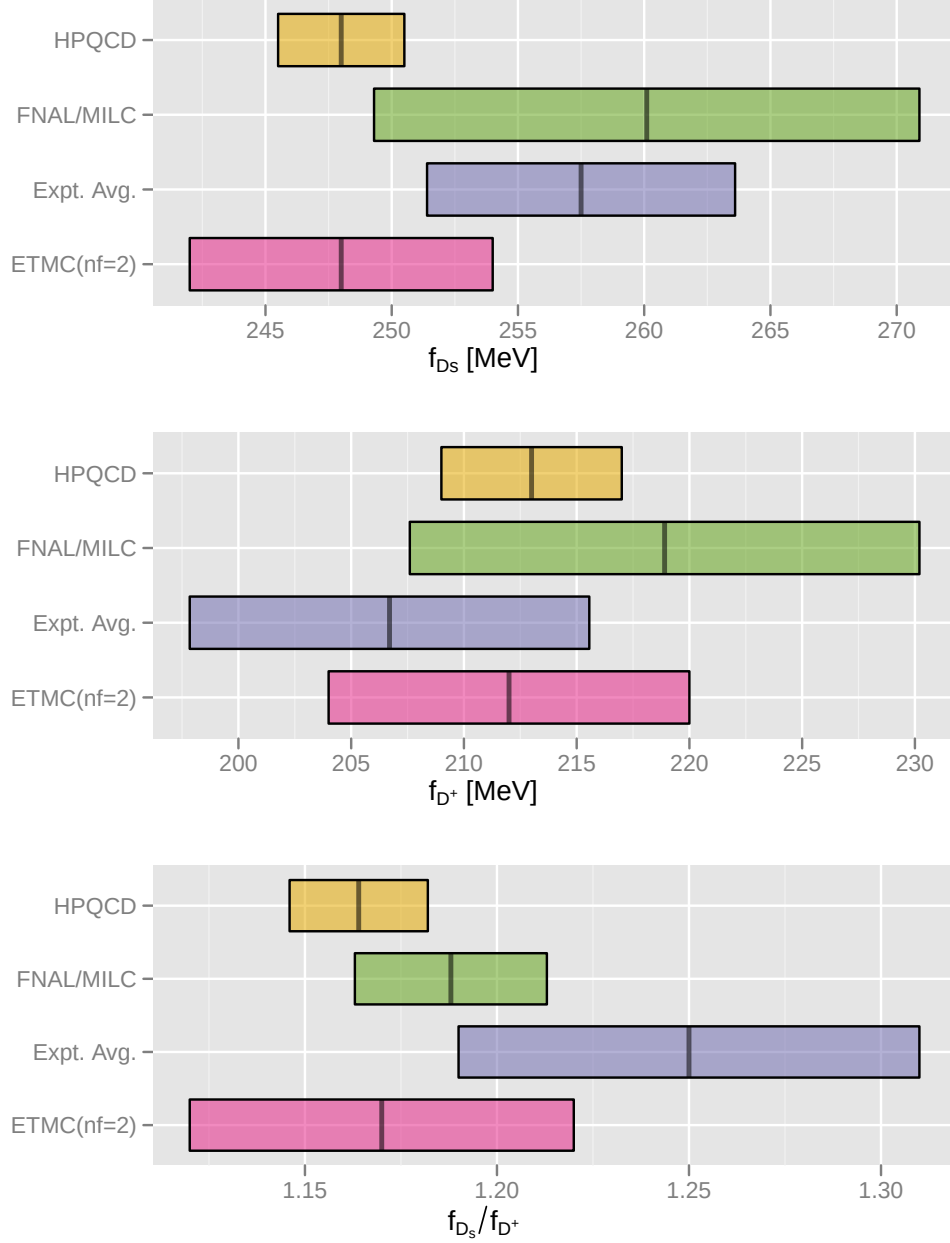


FIG. 12. Comparison of f_D and f_{D_s} with other two- and three-flavor lattice QCD calculations and with experiment. Results shown come from Refs. [50, 95–102]. The HPQCD f_D value is computed from their update to f_{D_s} and their earlier result for the ratio f_{D_s}/f_D .

While completing this analysis, we have begun runs to generate data that will address the main sources of uncertainty reported here. The new data set will contain four times the configurations used here to reduce the statistical errors in the correlation functions and, thus, directly improve the decay amplitudes, the determinations of the hopping-parameters

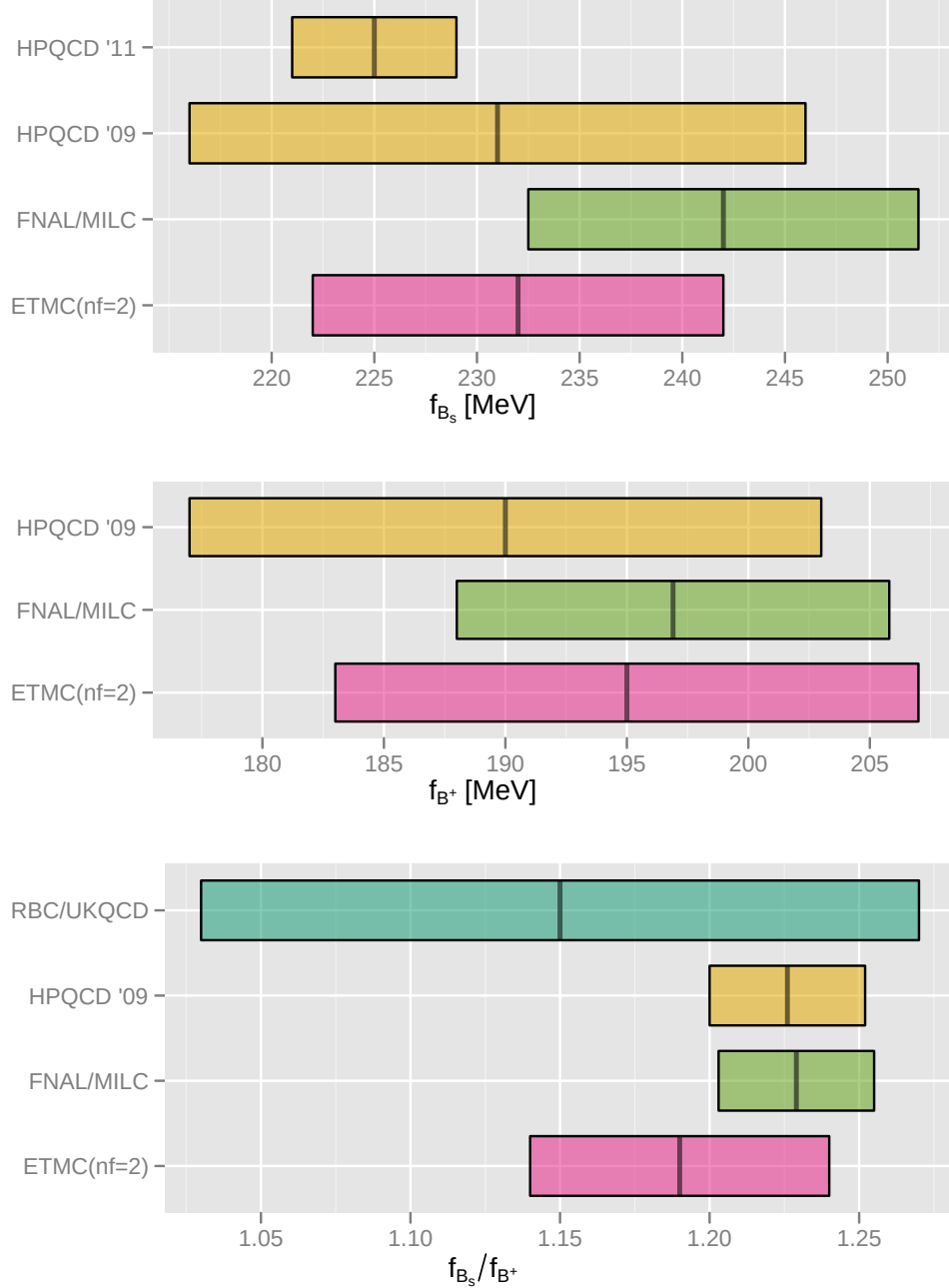


FIG. 13. Comparison of f_B and f_{B_s} with other two- and three-flavor lattice QCD calculations. Results shown come from Refs. [96, 104–106]. In the case of f_{B_s} HPQCD has two separate calculations using NRQCD b quarks and using HISQ b quarks; we show both the published NRQCD result (HPQCD '09) and the more recent HISQ result (HPQCD '11) in the plot above.

κ_c and κ_b , and the renormalization factors $Z_{V_{qq}^4}$ and $Z_{V_{QQ}^4}$, all of which feed into the decay constant. Our new data will also encompass two finer lattice spacings of $a \approx 0.06$ fm and $a \approx 0.045$ fm, in order to explicitly reduce light- and heavy-quark discretization errors and better control the continuum extrapolation. With four lattice spacings, our new method of heavy-quark discretization priors will be put to a more stringent test. The new runs will also include light valence- and sea-quark masses down to $\sim m_s/20$ in order to better control the chiral extrapolation to the physical d and u quark masses.

In order to reduce errors further, we will have to eliminate the errors from the matching factors and from quenching the charmed quark. The MILC Collaboration [107] is generating ensembles with 2+1+1 flavors of sea quarks with the HISQ action, with plans to provide a range of lattice spacings and sea quark masses equal to or more extensive than the 2+1 asqtad ensembles. Use of the HISQ action for the charm valence quark will allow us to further reduce many of the uncertainties, and provides the particularly nice advantage that one can use the local pseudoscalar density without multiplicative renormalization to obtain the continuum matrix element [108]. In several years, once the full suite of HISQ ensembles with several sea-quark masses and lattice spacings has been analyzed, we expect to obtain percent-level errors for both B - and D -meson decay constants. This will enable precise tests of the Standard Model and may help to reveal the presence of new physics in the quark-flavor sector.

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Appendix A: Heavy-quark Discretization Effects

We are using the heavy-quark Lagrangian as given in [33], with $\kappa_t = \kappa_s$ (or, equivalently, $\zeta = 1$), $r_s = 1$, and $c_B = c_E = c_{\text{SW}}$. This amounts to the Sheikholeslami-Wohlert Lagrangian [32] for Wilson fermions [59]. The current has a heavy quark of this type, rotated as in Eq. (4.2) (*cf.* Eqs. (7.8)–(7.10) of Ref. [33]), and a staggered light quark. At the tree level, the heavy-quark rotation is the same no matter what the other quark is. The discretization effects are estimated from a (continuum) effective field theory [36–38], as shown explicitly for decay constants in Eqs. (8.7)–(8.12) of Ref. [36].

1. Theory

Both QCD and lattice gauge theory can be described via

$$\mathcal{L}_{\text{QCD}} \doteq \mathcal{L}_{\text{HQET}} = \sum_i \mathcal{C}_i^{\text{cont}}(m_Q) \mathcal{O}_i, \quad (\text{A1})$$

$$\mathcal{L}_{\text{LGT}} \doteq \mathcal{L}_{\text{HQET}(m_0a)} = \sum_i \mathcal{C}_i^{\text{lat}}(m_Q, m_0a) \mathcal{O}_i, \quad (\text{A2})$$

where the $\mathcal{C}_i$ are short-distance coefficients and the $\mathcal{O}_i$ are operators describing the long-distance physics. The coefficients have dimension $4 - \dim \mathcal{O}_i$. For lattice gauge theory, they depend on m_0a , which is a ratio of short distances a and $1/m_Q$. The effective-theory operators $\mathcal{O}_i$ in Eqs. (A1) and (A2) are the same.

The error from each term is simply the difference

$$\text{error}_i = |[\mathcal{C}_i^{\text{lat}}(m_Q, m_0a) - \mathcal{C}_i^{\text{cont}}(m_Q)] \mathcal{O}_i|. \quad (\text{A3})$$

The relative error in our matrix elements can be estimated by setting $\langle \mathcal{O}_i \rangle \sim \Lambda_{\text{QCD}}^{\dim \mathcal{O}_i - 4}$; choices for the QCD scale Λ_{QCD} are discussed below. The coefficient mismatch can be written

$$\mathcal{C}_i^{\text{lat}}(m_Q, m_0a) - \mathcal{C}_i^{\text{cont}}(m_Q) = a^{\dim \mathcal{O}_i - 4} f_i(m_0a). \quad (\text{A4})$$

This recovers the usual counting of powers of a (familiar from Symanzik [34, 35]), but maintaining the full m_0a dependence. The final expression for the discretization errors is then

$$\text{error}_i \propto f_i(m_0a) (a\Lambda_{\text{QCD}})^{\dim \mathcal{O}_i - 4}. \quad (\text{A5})$$

For Wilson fermions, $\lim_{m_0a \rightarrow 0} f_i = \text{constant}$ (whereas in lattice NRQCD without fine tuning this is not the case). We have explicit calculations of the f_i for the $O(a)$ and $O(a^2)$ errors at the tree level [33, 60]. The next subsection discusses how to use them to guide a continuum-limit extrapolation the $O(\alpha_s a)$ and $O(a^2)$ errors.

Equations (A1) and (A2) can be generalized to currents. For the axial-vector current,

$$\mathcal{A}^\mu \doteq C_{A\perp}^{\text{cont}}(m_Q) \bar{q} i \gamma_\perp^\mu \gamma_5 h_v - C_{A\parallel}^{\text{cont}}(m_Q) v^\mu \bar{q} \gamma_5 h_v - \sum_i B_{Ai}^{\text{cont}}(m_Q) \mathcal{Q}_{Ai}^\mu, \quad (\text{A6})$$

$$A_{\text{lat}}^\mu \doteq C_{A\perp}^{\text{lat}}(m_Q, m_0a) \bar{q} i \gamma_\perp^\mu \gamma_5 h_v - C_{A\parallel}^{\text{lat}}(m_Q, m_0a) v^\mu \bar{q} \gamma_5 h_v - \sum_i B_{Ai}^{\text{lat}}(m_Q, m_0a) \mathcal{Q}_{Ai}^\mu, \quad (\text{A7})$$

and $\doteq$ again means in the sense of matrix elements. Here v^μ selects the temporal component and $\perp$ the spatial, and the list of dimension-4 operators $\mathcal{Q}$ can be found in Refs. [37].

The matrix element of the temporal component of the axial-vector current [*cf.* Eq. (4.7)] is normalized by multiplying with $Z_{A^4} = C_{A\parallel}^{\text{cont}}/C_{A\parallel}^{\text{lat}}$. The current mismatch then leads to errors

$$a^{\dim \mathcal{Q}_i - 3} f_i(m_0 a) = Z_{A^4} B_{Ai}^{\text{lat}} - B_{Ai}^{\text{cont}}, \quad (\text{A8})$$

with the sum running over the two operators $\mathcal{Q}$ that point in the temporal direction [37].

2. Error Estimation

The total error from heavy-quark discretization effects is then

$$\text{error} = \sum_i z_i (a\Lambda_{\text{QCD}})^{s_i} f_i(m_0 a) \quad (\text{A9})$$

where the sum runs over Lagrangian operators $\mathcal{O}_i$ of dimension 5 and 6 and current operators $\mathcal{Q}_i$ of dimension 4 and 5, $s_i = \dim \mathcal{O}_i - 4$ or $\dim \mathcal{Q}_i - 3$, and the z_i are unknown coefficients. The functions f_i (summarized below) have been computed for $\mathcal{O}(a^2)$ and estimated for $\mathcal{O}(\alpha_s a)$. We omit contributions of order $\alpha_s^l a^2$, whether from extra operators or from iterating to second order operators with coefficients of order $\alpha_s a$.

In the past, we have taken a very conservative $\Lambda_{\text{QCD}} = 700$ MeV and assumed a Gaussian distribution for the z_i centered on 0 and of width 1. This amounts to treating the discretization errors as independent and adding them in quadrature. It also implicitly assumes that the data have nothing to say about the size or relative importance of the terms.

Here, however, we incorporate these errors into the chiral-continuum extrapolation, discussed in Sec. VI. This means that the z_i are now constrained fit parameters, with prior constraints discussed in Sec. VI.

The f_i are collected next.

a. $\mathcal{O}(a^2)$ errors

We start with these, because explicit expressions for the functions $f_i(m_0 a)$ are available. The Lagrangian leads to two bilinears, $\bar{h}\mathbf{D} \cdot \mathbf{E}h$ and $\bar{h}i\mathbf{\Sigma} \cdot [\mathbf{D} \times \mathbf{E}]h$, and many four-quark operators. At the tree level the coefficients of all four-quark operators vanish. At the tree level the coefficients of the two bilinears are the same, and the mismatch function is

$$f_E(m_0 a) = \frac{1}{8m_E^2 a^2} - \frac{1}{2(2m_2 a)^2}. \quad (\text{A10})$$

Using explicit expressions for $1/m_2$ [33] and $1/m_E^2$ [60], one finds

$$f_E(m_0 a) = \frac{1}{2} \left[\frac{c_E(1 + m_0 a) - 1}{m_0 a(2 + m_0 a)(1 + m_0 a)} - \frac{1}{4(1 + m_0 a)^2} \right]. \quad (\text{A11})$$

We are using $c_E = 1$, so

$$f_E(m_0 a) = \frac{2 + 3m_0 a}{8(2 + m_0 a)(1 + m_0 a)^2}. \quad (\text{A12})$$

With no further assumptions, this term enters twice independently, so we take the width of this prior to be $\sqrt{2}$ rather than 1.

The current leads to three more terms with non-zero coefficients, $\bar{q}\Gamma\mathbf{D}^2h$, $\bar{q}\Gamma i\mathbf{\Sigma}\cdot\mathbf{B}h$, and $\bar{q}\Gamma\mathbf{\alpha}\cdot\mathbf{E}h$, which can be deduced from Eq. (A17) of Ref. [33]. Their coefficients can be read off from Eq. (A19). When $c_B = r_s$ the first two share the same coefficient

$$\begin{aligned} f_X(m_0a) &= \frac{1}{8m_X^2a^2} - \frac{\zeta d_1(1+m_0a)}{m_0a(2+m_0a)} - \frac{1}{2(2m_2a)^2}, \\ &= \frac{1}{2} \left[\frac{1}{(2+m_0a)(1+m_0a)} + \frac{1}{2(1+m_0a)} - \frac{1}{4(1+m_0a)^2} - \frac{1}{(2+m_0a)^2} \right], \\ &= \frac{1}{2} \left[\frac{1}{2(1+m_0a)} - \left(\frac{m_0a}{2(2+m_0a)(1+m_0a)} \right)^2 \right], \end{aligned} \quad (\text{A13})$$

where the last term on the second line comes from using the tree-level d_1 (as we do in the simulations). Because of the two-fold appearance, we again take the prior width to be $\sqrt{2}$.

For $\bar{q}\Gamma\mathbf{\alpha}\cdot\mathbf{E}h$

$$\begin{aligned} f_Y(m_0a) &= \frac{1}{2} \left[\frac{d_1}{m_2a} - \frac{\zeta(1-c_E)(1+m_0a)}{m_0a(2+m_0a)} \right], \\ &= \frac{2+4m_0a+(m_0a)^2}{4(1+m_0a)^2(2+m_0a)^2}, \end{aligned} \quad (\text{A14})$$

where the last line reflects the choices made for c_E and d_1 .

b. $O(\alpha_s a)$ and $O(a^3)$ errors

Here the mismatch functions $f_i(m_0a)$ start at order α_s , and we do not have explicit expressions for them. We take unimproved tree-level coefficients as a guide to the combinatoric factors and the asymptotic behavior as $m_0a \rightarrow 0$ and $m_0a \rightarrow \infty$.

The Lagrangian leads to two bilinears, the kinetic energy $\mathcal{O}_2 = \bar{h}\mathbf{D}^2h$ and the chromomagnetic moment $\mathcal{O}_B = \bar{h}i\mathbf{\Sigma}\cdot\mathbf{B}h$. We match the former nonperturbatively, by identifying the meson's kinetic mass with the physical mass; the discretization error f_2 stems, therefore, from discretization effects in M_2 .

The computed kinetic meson mass is

$$M_2 = m_2(\kappa) + \text{continuum binding energy} + \delta M_2, \quad (\text{A15})$$

where [55]

$$\delta M_2 = \frac{\bar{\Lambda}^2}{6m_Q} \left[5 \left(\frac{m_2^3}{m_4^3} - 1 \right) + 4w_4(m_2a)^3 \right], \quad (\text{A16})$$

and m_2 , m_4 , and w_4 are functions of m_0a and, hence, κ . (See Refs. [33, 60] for explicit expressions.) Equating M_2 to a physical meson mass means that we choose κ such that $m_2(\kappa) + \delta M_2 = m_Q$, thereby making in ϕ a relative error

$$\text{error}_2 = \bar{\Lambda} \left(\frac{1}{2m_2} - \frac{1}{2m_Q} \right) = \bar{\Lambda} \left(\frac{1}{2m_Q - 2\delta M_2} - \frac{1}{2m_Q} \right) \approx \bar{\Lambda} \frac{\delta M_2}{2m_Q^2}. \quad (\text{A17})$$

The right-most expression is $(a\bar{\Lambda})^3 f_2(m_0a)$, $f_2 = []/12(m_2a)^3$, where $[]$ is the bracket in Eq. (A16). It is formally smaller than the other errors considered here— f_2 is of order 1 for all m_0a . Numerically, however, it is not much smaller.

At the tree level the chromomagnetic mismatch is

$$f_B^{[0]}(m_0 a) = \frac{c_B - 1}{2(1 + m_0 a)}. \quad (\text{A18})$$

This has the right asymptotic behavior in both limits, so our Ansatz for the one-loop mismatch function is simply

$$f_B(m_0 a) = \frac{\alpha_s}{2(1 + m_0 a)}, \quad (\text{A19})$$

and error_B is this function multiplied by $a\Lambda$. We take $\alpha_s = 0.288$ on the $a \approx 0.12$ fm ensembles, which is the value determined for α_V from the plaquette [76] with one-loop running to scale $q^* = 2.5/a$. On other ensembles, α_s is found by assuming that the measured average taste splitting goes like $\alpha_s^2 a^2$ (with a determined from r_1/a). This gives α_s values that track $\alpha_V(q^* = 2.5/a)$ quite well, which is why we make that q^* choice. The results are rather insensitive to the details here. For example, using $\alpha_s = 0.325$ on the $a \approx 0.12$ fm ensembles, which corresponds to $q^* = 2.0/a$, increases the error estimate by less than 0.6 MeV for f_{D^+} , and less than 0.25 MeV for f_{B^+} .

The current leads to one more term, with tree-level mismatch function

$$f_3^{[0]}(m_0 a) = \frac{m_0 a}{2(2 + m_0 a)(1 + m_0 a)} - d_1, \quad (\text{A20})$$

and the tree-level d_1 is chosen so that $f_3^{[0]} = 0$. As with the mismatch function f_B , we would like to anticipate $f_3^{[1]}$ by setting $d_1^{[1]} = 0$ and multiplying the rest with α_s . But it is not generic that this vanishes as $m_0 a \rightarrow 0$. Therefore, we take

$$f_3(m_0 a) = \frac{\alpha_s}{2(2 + m_0 a)}, \quad (\text{A21})$$

which has the right asymptotic behavior. We take the prior width as $\sqrt{2}$, because A^4 has two such corrections [37].

3. Dispersion relation, Eq. (3.1)

We take a similar approach to the dispersion relation, Eq. (3.1), with the difference that we now know the sign of the leading effect.

The tree-level functions are

$$a_4^{[0]} = \frac{1}{(m_2^{[0]} a)^2} - \frac{m_1^{[0]} a}{(m_4^{[0]} a)^3}, \quad (\text{A22})$$

$$a_{4'}^{[0]} = m_1^{[0]} a w_4^{[0]}. \quad (\text{A23})$$

The binding energy enters A_4 and $A_{4'}$ via the meson's kinetic energy. Hence, the binding contributions are

$$A'_4 = \frac{3m_1^{[0]} a}{m_2^{[0]} a (m_4^{[0]} a)^3} - \frac{2}{(m_2^{[0]} a)^3} - \frac{1}{(m_4^{[0]} a)^3}, \quad (\text{A24})$$

$$A'_{4'} = w_4^{[0]} \left(1 - \frac{m_1^{[0]} a}{m_2^{[0]} a} \right), \quad (\text{A25})$$

and in Eq. (3.4) the binding energy floats within a Gaussian prior described by $(\bar{\Lambda}, \sigma_{\bar{\Lambda}}) = (600, 400)$ MeV. This choice conservatively brackets the binding energy of a heavy-strange meson. For the higher-order perturbative contribution to the coefficients, we take the Ansätze based on the asymptotic behavior:

$$a_4^{[1]} = \frac{y_4 + z_4 \ln(1 + m_0 a)}{(1 + m_0 a)^2}, \quad (\text{A26})$$

$$a_{4'}^{[1]} = \frac{y_{4'} m_0 a + z_{4'} \ln(1 + m_0 a)}{1 + m_0 a}, \quad (\text{A27})$$

where the y s and z s float within Gaussian priors described by $(y_4, \sigma_{y_4}) = (3, 5)$, $(z_4, \sigma_{z_4}) = (1, 2)$, $(y_{4'}, \sigma_{y_{4'}}) = (0, 0)$, and $(z_{4'}, \sigma_{z_{4'}}) = (0, 2)$. The terms proportional to y_i stem from the $m_0 a \rightarrow 0$ limit, in which the renormalization of m_4 must coincide with that of m_1 , and $a_4 = m_1 a w_4$ must vanish like $m_0 a$. The terms proportional to z_i stem from the $m_0 a \rightarrow \infty$ limit, where the static limit is obtained. Except for $y_{4'}$, the numerical values have been chosen consistent with one-loop experience for m_1 and m_2 [109]. We have set $y_{4'} \equiv 0$, because at small $m_0 a$ it is indistinguishable from the other term in $a_{4'}^{[1]}$, and our range of $m_0 a$ does not reach far into the region $m_0 a \gg 1$.

Appendix B: Two point fit results from Analysis I

TABLE XIV. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from Analysis I fits of the charm correlators at lattice spacing $a \approx 0.09$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0031/0.031	0.0031	0.7523(0.0016)	0.0857(0.0015)	58/48	0.23
0.0031/0.031	0.0044	0.7553(0.0014)	0.0873(0.0013)	56/48	0.28
0.0031/0.031	0.0062	0.7589(0.0011)	0.0890(0.0011)	55/48	0.33
0.0031/0.031	0.0087	0.7634(0.0009)	0.0910(0.0009)	53/48	0.38
0.0031/0.031	0.0124	0.7699(0.0007)	0.0936(0.0007)	53/48	0.41
0.0031/0.031	0.0186	0.7807(0.0005)	0.0978(0.0006)	52/48	0.44
0.0031/0.031	0.0272	0.7954(0.0004)	0.1030(0.0005)	50/48	0.5
0.0031/0.031	0.031	0.8018(0.0004)	0.1052(0.0004)	50/48	0.5
0.0062/0.031	0.0031	0.7541(0.0030)	0.0875(0.0027)	56/48	0.37
0.0062/0.031	0.0044	0.7577(0.0023)	0.0899(0.0021)	52/48	0.49
0.0062/0.031	0.0062	0.7613(0.0019)	0.0917(0.0018)	50/48	0.58
0.0062/0.031	0.0087	0.7654(0.0015)	0.0933(0.0015)	58/51	0.43
0.0062/0.031	0.0124	0.7712(0.0012)	0.0952(0.0012)	52/48	0.48
0.0062/0.031	0.0186	0.7810(0.0009)	0.0985(0.0010)	56/48	0.37
0.0062/0.031	0.0272	0.7952(0.0006)	0.1032(0.0008)	59/48	0.28
0.0062/0.031	0.031	0.8015(0.0005)	0.1052(0.0007)	60/48	0.25
0.0124/0.031	0.0031	0.7551(0.0038)	0.0930(0.0036)	60/48	0.27
0.0124/0.031	0.0042	0.7554(0.0031)	0.0926(0.0028)	65/48	0.15
0.0124/0.031	0.0062	0.7574(0.0023)	0.0929(0.0021)	65/48	0.16
0.0124/0.031	0.0087	0.7608(0.0017)	0.0938(0.0015)	59/48	0.28
0.0124/0.031	0.0124	0.7666(0.0013)	0.0957(0.0012)	49/48	0.63
0.0124/0.031	0.0186	0.7766(0.0008)	0.0991(0.0009)	42/48	0.85
0.0124/0.031	0.0272	0.7907(0.0006)	0.1038(0.0007)	48/48	0.64
0.0124/0.031	0.031	0.7969(0.0005)	0.1058(0.0006)	53/48	0.47

TABLE XV. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from Analysis I fits of the charm correlators at lattice spacing $a \approx 0.12$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.005/0.050	0.005	0.9943(0.0032)	0.1436(0.0030)	30/30	0.52
0.005/0.050	0.007	0.9977(0.0024)	0.1453(0.0024)	29/30	0.6
0.005/0.050	0.01	1.0026(0.0018)	0.1477(0.0019)	28/30	0.64
0.005/0.050	0.014	1.0090(0.0016)	0.1508(0.0017)	28/30	0.64
0.005/0.050	0.02	1.0186(0.0013)	0.1551(0.0015)	29/30	0.58
0.005/0.050	0.03	1.0345(0.0010)	0.1620(0.0012)	33/30	0.42
0.005/0.050	0.0415	1.0526(0.0008)	0.1694(0.0010)	36/30	0.27
0.007/0.050	0.005	0.9948(0.0035)	0.1442(0.0035)	17/30	0.98
0.007/0.050	0.007	0.9975(0.0027)	0.1455(0.0028)	19/30	0.95
0.007/0.050	0.01	1.0019(0.0021)	0.1476(0.0021)	22/30	0.89
0.007/0.050	0.014	1.0081(0.0016)	0.1504(0.0017)	24/30	0.83
0.007/0.050	0.02	1.0178(0.0012)	0.1547(0.0014)	23/30	0.85
0.007/0.050	0.03	1.0338(0.0009)	0.1615(0.0010)	20/30	0.94
0.007/0.050	0.0415	1.0520(0.0007)	0.1687(0.0008)	19/30	0.95
0.010/0.050	0.005	0.9958(0.0039)	0.1461(0.0041)	15/30	0.99
0.010/0.050	0.007	1.0000(0.0031)	0.1486(0.0032)	20/30	0.94
0.010/0.050	0.01	1.0057(0.0024)	0.1516(0.0026)	26/30	0.75
0.010/0.050	0.014	1.0126(0.0019)	0.1549(0.0021)	29/27	0.41
0.010/0.050	0.02	1.0226(0.0015)	0.1594(0.0017)	33/30	0.39
0.010/0.050	0.03	1.0387(0.0011)	0.1662(0.0014)	31/30	0.5
0.010/0.050	0.0415	1.0567(0.0008)	0.1733(0.0011)	27/30	0.68
0.020/0.050	0.005	0.9942(0.0046)	0.1537(0.0050)	49/30	0.036
0.020/0.050	0.007	0.9959(0.0036)	0.1533(0.0039)	49/30	0.036
0.020/0.050	0.01	0.9987(0.0027)	0.1532(0.0031)	48/30	0.051
0.020/0.050	0.014	1.0037(0.0021)	0.1543(0.0024)	45/30	0.075
0.020/0.050	0.02	1.0124(0.0016)	0.1575(0.0019)	43/30	0.11
0.020/0.050	0.03	1.0274(0.0011)	0.1632(0.0014)	37/30	0.27
0.020/0.050	0.0415	1.0447(0.0009)	0.1695(0.0012)	32/30	0.48
0.030/0.050	0.005	0.9830(0.0042)	0.1475(0.0042)	33/30	0.39
0.030/0.050	0.007	0.9853(0.0033)	0.1485(0.0033)	33/30	0.4
0.030/0.050	0.01	0.9897(0.0025)	0.1505(0.0025)	32/30	0.47
0.030/0.050	0.014	0.9960(0.0020)	0.1534(0.0020)	31/30	0.53
0.030/0.050	0.02	1.0054(0.0015)	0.1574(0.0016)	32/30	0.46
0.030/0.050	0.03	1.0205(0.0011)	0.1633(0.0012)	37/30	0.27
0.030/0.050	0.0415	1.0376(0.0009)	0.1695(0.0010)	40/30	0.15

TABLE XVI. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from Analysis I fits of the charm correlators at lattice spacing $a \approx 0.15$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0097/0.0484	0.0048	1.1659(0.0044)	0.1979(0.0052)	20/20	0.5
0.0097/0.0484	0.007	1.1710(0.0034)	0.2017(0.0040)	22/20	0.37
0.0097/0.0484	0.0097	1.1768(0.0027)	0.2054(0.0032)	25/20	0.26
0.0097/0.0484	0.0194	1.1951(0.0016)	0.2159(0.0020)	25/20	0.26
0.0097/0.0484	0.029	1.2117(0.0012)	0.2242(0.0015)	20/20	0.51
0.0097/0.0484	0.0484	1.2432(0.0009)	0.2385(0.0012)	15/20	0.79
0.0194/0.0484	0.0048	1.1726(0.0046)	0.2106(0.0052)	23/20	0.35
0.0194/0.0484	0.007	1.1749(0.0036)	0.2105(0.0041)	23/20	0.35
0.0194/0.0484	0.0097	1.1785(0.0028)	0.2113(0.0031)	23/20	0.32
0.0194/0.0484	0.0194	1.1935(0.0016)	0.2174(0.0020)	30/20	0.092
0.0194/0.0484	0.029	1.2091(0.0013)	0.2244(0.0016)	32/20	0.055
0.0194/0.0484	0.0484	1.2400(0.0010)	0.2381(0.0013)	27/20	0.17
0.0290/0.0484	0.0048	1.1613(0.0044)	0.1975(0.0049)	17/20	0.72
0.0290/0.0484	0.007	1.1660(0.0034)	0.2010(0.0040)	18/20	0.64
0.0290/0.0484	0.0097	1.1717(0.0026)	0.2049(0.0031)	21/20	0.47
0.0290/0.0484	0.0194	1.1896(0.0015)	0.2151(0.0019)	24/20	0.3
0.0290/0.0484	0.029	1.2058(0.0011)	0.2229(0.0015)	23/20	0.32
0.0290/0.0484	0.0484	1.2368(0.0008)	0.2364(0.0011)	20/20	0.49

TABLE XVII. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from Analysis I fits of the bottom correlators at lattice spacing $a \approx 0.09$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0031/0.031	0.0031	1.6509(0.0018)	0.1359(0.0016)	41/39	0.48
0.0031/0.031	0.0044	1.6532(0.0016)	0.1378(0.0015)	40/39	0.51
0.0031/0.031	0.0062	1.6562(0.0015)	0.1402(0.0014)	40/39	0.49
0.0031/0.031	0.0087	1.6601(0.0013)	0.1433(0.0014)	42/39	0.42
0.0031/0.031	0.0124	1.6659(0.0012)	0.1475(0.0013)	45/39	0.31
0.0031/0.031	0.0186	1.6752(0.0011)	0.1542(0.0012)	47/39	0.23
0.0031/0.031	0.0272	1.6879(0.0009)	0.1628(0.0011)	49/39	0.19
0.0031/0.031	0.031	1.6934(0.0009)	0.1664(0.0011)	49/39	0.18
0.0062/0.031	0.0031	1.6539(0.0046)	0.1358(0.0051)	40/39	0.56
0.0062/0.031	0.0044	1.6557(0.0039)	0.1377(0.0044)	37/39	0.68
0.0062/0.031	0.0062	1.6584(0.0032)	0.1402(0.0037)	34/39	0.77
0.0062/0.031	0.0087	1.6620(0.0027)	0.1434(0.0031)	34/39	0.8
0.0062/0.031	0.0124	1.6675(0.0022)	0.1480(0.0026)	36/39	0.72
0.0062/0.031	0.0186	1.6767(0.0018)	0.1550(0.0022)	41/39	0.53
0.0062/0.031	0.0272	1.6892(0.0014)	0.1637(0.0019)	45/39	0.37
0.0062/0.031	0.031	1.6946(0.0014)	0.1672(0.0018)	45/39	0.35
0.0124/0.031	0.0031	1.6532(0.0036)	0.1387(0.0038)	52/39	0.16
0.0124/0.031	0.0042	1.6550(0.0033)	0.1407(0.0034)	48/39	0.27
0.0124/0.031	0.0062	1.6576(0.0030)	0.1432(0.0031)	40/39	0.55
0.0124/0.031	0.0087	1.6606(0.0027)	0.1456(0.0029)	35/39	0.77
0.0124/0.031	0.0124	1.6650(0.0024)	0.1488(0.0027)	33/39	0.84
0.0124/0.031	0.0186	1.6730(0.0019)	0.1544(0.0023)	36/39	0.73
0.0124/0.031	0.0272	1.6847(0.0016)	0.1623(0.0021)	42/39	0.48
0.0124/0.031	0.031	1.6900(0.0015)	0.1657(0.0020)	45/39	0.38

TABLE XVIII. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from Analysis I fits of the bottom correlators at lattice spacing $a \approx 0.12$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.005/0.050	0.005	1.9170(0.0044)	0.2236(0.0050)	45/27	0.03
0.005/0.050	0.007	1.9197(0.0039)	0.2263(0.0046)	46/27	0.022
0.005/0.050	0.01	1.9235(0.0033)	0.2300(0.0040)	46/27	0.021
0.005/0.050	0.014	1.9287(0.0029)	0.2347(0.0036)	45/27	0.027
0.005/0.050	0.02	1.9367(0.0024)	0.2418(0.0031)	43/27	0.046
0.005/0.050	0.03	1.9503(0.0020)	0.2532(0.0026)	39/27	0.096
0.005/0.050	0.0415	1.9657(0.0017)	0.2654(0.0023)	36/27	0.17
0.007/0.050	0.005	1.9147(0.0036)	0.2224(0.0039)	37/27	0.12
0.007/0.050	0.007	1.9177(0.0033)	0.2254(0.0037)	35/27	0.17
0.007/0.050	0.01	1.9219(0.0030)	0.2292(0.0036)	34/27	0.2
0.007/0.050	0.014	1.9272(0.0028)	0.2337(0.0037)	35/27	0.19
0.007/0.050	0.02	1.9351(0.0026)	0.2401(0.0037)	36/27	0.15
0.007/0.050	0.03	1.9485(0.0022)	0.2508(0.0035)	38/27	0.096
0.007/0.050	0.0415	1.9638(0.0019)	0.2628(0.0031)	40/27	0.07
0.010/0.050	0.005	1.9182(0.0047)	0.2254(0.0047)	30/27	0.4
0.010/0.050	0.007	1.9207(0.0041)	0.2284(0.0042)	32/27	0.29
0.010/0.050	0.01	1.9250(0.0035)	0.2328(0.0037)	36/27	0.18
0.010/0.050	0.014	1.9307(0.0030)	0.2383(0.0033)	39/27	0.097
0.010/0.050	0.02	1.9391(0.0025)	0.2457(0.0028)	43/27	0.048
0.010/0.050	0.03	1.9527(0.0020)	0.2569(0.0024)	47/27	0.02
0.010/0.050	0.0415	1.9682(0.0017)	0.2689(0.0021)	51/27	0.0092
0.020/0.050	0.005	1.9136(0.0060)	0.2278(0.0069)	33/27	0.27
0.020/0.050	0.007	1.9163(0.0050)	0.2305(0.0059)	33/27	0.28
0.020/0.050	0.01	1.9200(0.0042)	0.2340(0.0050)	31/27	0.36
0.020/0.050	0.014	1.9249(0.0036)	0.2381(0.0043)	29/27	0.47
0.020/0.050	0.02	1.9322(0.0031)	0.2437(0.0039)	28/27	0.52
0.020/0.050	0.03	1.9445(0.0027)	0.2526(0.0038)	30/27	0.42
0.020/0.050	0.0415	1.9590(0.0025)	0.2627(0.0039)	33/27	0.3
0.030/0.050	0.005	1.9030(0.0058)	0.2196(0.0073)	38/27	0.12
0.030/0.050	0.007	1.9058(0.0049)	0.2223(0.0064)	32/27	0.29
0.030/0.050	0.01	1.9099(0.0041)	0.2258(0.0056)	27/27	0.56
0.030/0.050	0.014	1.9155(0.0034)	0.2306(0.0048)	23/27	0.74
0.030/0.050	0.02	1.9239(0.0028)	0.2376(0.0040)	22/27	0.77
0.030/0.050	0.03	1.9372(0.0022)	0.2479(0.0034)	25/27	0.64
0.030/0.050	0.0415	1.9518(0.0019)	0.2585(0.0032)	28/27	0.49

TABLE XIX. Heavy-light pseudoscalar meson masses and renormalized decay amplitudes obtained from Analysis I fits of the bottom correlators at lattice spacing $a \approx 0.15$ fm.

am_l/am_s	am_q	aM_H	$a^{3/2}\phi_H$	χ^2/dof	p
0.0097/0.0484	0.0048	2.2553(0.0071)	0.3311(0.0115)	36/25	0.097
0.0097/0.0484	0.007	2.2576(0.0061)	0.3341(0.0102)	37/25	0.09
0.0097/0.0484	0.0097	2.2611(0.0052)	0.3389(0.0089)	36/25	0.1
0.0097/0.0484	0.0194	2.2757(0.0036)	0.3568(0.0063)	34/25	0.16
0.0097/0.0484	0.029	2.2901(0.0030)	0.3727(0.0053)	33/25	0.16
0.0097/0.0484	0.0484	2.3175(0.0023)	0.4002(0.0046)	35/25	0.12
0.0194/0.0484	0.0048	2.2296(0.0175)	0.2743(0.0416)	32/25	0.2
0.0194/0.0484	0.007	2.2349(0.0142)	0.2823(0.0357)	34/25	0.15
0.0194/0.0484	0.0097	2.2416(0.0118)	0.2917(0.0309)	36/25	0.1
0.0194/0.0484	0.0194	2.2639(0.0072)	0.3243(0.0202)	36/25	0.1
0.0194/0.0484	0.029	2.2819(0.0054)	0.3482(0.0152)	30/25	0.27
0.0194/0.0484	0.0484	2.3124(0.0038)	0.3839(0.0109)	24/25	0.59
0.0290/0.0484	0.0048	2.2402(0.0073)	0.3101(0.0123)	29/25	0.32
0.0290/0.0484	0.007	2.2464(0.0061)	0.3199(0.0104)	30/25	0.28
0.0290/0.0484	0.0097	2.2524(0.0052)	0.3289(0.0089)	31/25	0.25
0.0290/0.0484	0.0194	2.2695(0.0036)	0.3502(0.0066)	27/25	0.42
0.0290/0.0484	0.029	2.2847(0.0030)	0.3665(0.0058)	21/25	0.72
0.0290/0.0484	0.0484	2.3125(0.0025)	0.3939(0.0057)	18/25	0.87

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- [1] A. Lenz *et al.* (CKMfitter), *Phys. Rev.* **D83**, 036004 (2011), [arXiv:1008.1593 \[hep-ph\]](#)
 - [2] E. Lunghi and A. Soni, *Phys. Lett.* **B697**, 323 (2011), [arXiv:1010.6069 \[hep-ph\]](#)
 - [3] J. Laiho, E. Lunghi, and R. Van de Water, PoS **FPCP2010**, 040 (2010), [arXiv:1102.3917 \[hep-ph\]](#)
 - [4] K. Hara *et al.* (Belle), *Phys. Rev.* **D82**, 071101 (2010), [arXiv:1006.4201 \[hep-ex\]](#)
 - [5] P. del Amo Sanchez *et al.* (BaBar)(2010), [arXiv:1008.0104 \[hep-ex\]](#)
 - [6] M. Masuzawa, in *Proceedings of IPAC 2010*, edited by K. Oide (2010) <http://accelconf.web.cern.ch/AccelConf/IPAC10/>
 - [7] T. Iijima, “Search for Charged Higgs in $B \rightarrow \tau\nu$ and $D \rightarrow \tau\nu$ Decays,” (2009), <http://kds.kek.jp/materialDisplay.py?contribId=5&sessionId=2&materialId=slides&confId=2865>
 - [8] E. Lunghi and A. Soni, *Phys. Rev. Lett.* **104**, 251802 (2010), [arXiv:0912.0002 \[hep-ph\]](#)
 - [9] C. T. H. Davies *et al.* (HPQCD, MILC, and Fermilab Lattice), *Phys. Rev. Lett.* **92**, 022001 (2004), [arXiv:hep-lat/0304004](#)
 - [10] L. Susskind, *Phys. Rev.* **D16**, 3031 (1977)
 - [11] H. S. Sharatchandra, H. J. Thun, and P. Weisz, *Nucl. Phys.* **B192**, 205 (1981)
 - [12] C. Aubin *et al.* (MILC), *Phys. Rev.* **D70**, 114501 (2004), [arXiv:hep-lat/0407028 \[hep-lat\]](#)
 - [13] I. F. Allison *et al.* (HPQCD), *Phys. Rev. Lett.* **94**, 172001 (2005), [arXiv:hep-lat/0411027](#)
 - [14] S. Prelovšek, *Phys. Rev.* **D73**, 014506 (2006), [arXiv:hep-lat/0510080](#)
 - [15] C. Bernard, *Phys. Rev.* **D73**, 114503 (2006), [arXiv:hep-lat/0603011](#)
 - [16] C. Bernard, C. E. DeTar, Z. Fu, and S. Prelovšek, *Phys. Rev.* **D76**, 094504 (2007), [arXiv:0707.2402 \[hep-lat\]](#)
 - [17] C. Aubin, J. Laiho, and R. S. Van de Water, *Phys. Rev.* **D77**, 114501 (2008), [arXiv:0803.0129 \[hep-lat\]](#)
 - [18] C. Bernard, M. Golterman, and Y. Shamir, *Phys. Rev.* **D73**, 114511 (2006), [arXiv:hep-lat/0604017 \[hep-lat\]](#)
 - [19] Y. Shamir, *Phys. Rev.* **D71**, 034509 (2005), [arXiv:hep-lat/0412014](#)
 - [20] Y. Shamir, *Phys. Rev.* **D75**, 054503 (2007), [arXiv:hep-lat/0607007](#)
 - [21] C. Bernard, M. Golterman, and Y. Shamir, *Phys. Rev.* **D77**, 074505 (2008), [arXiv:0712.2560 \[hep-lat\]](#)
 - [22] W.-J. Lee and S. R. Sharpe, *Phys. Rev.* **D60**, 114503 (1999), [arXiv:hep-lat/9905023](#)
 - [23] C. Aubin and C. Bernard, *Phys. Rev.* **D68**, 034014 (2003), [hep-lat/0304014](#)
 - [24] S. R. Sharpe and R. S. Van de Water, *Phys. Rev.* **D71**, 114505 (2005), [arXiv:hep-lat/0409018](#)
 - [25] S. R. Sharpe, PoS **LAT2006**, 022 (2006), [arXiv:hep-lat/0610094](#)
 - [26] A. S. Kronfeld, PoS **LAT2007**, 016 (2007), [arXiv:0711.0699 \[hep-lat\]](#)
 - [27] M. Golterman, PoS **CONFINEMENT8**, 014 (2008), [arXiv:0812.3110 \[hep-ph\]](#)
 - [28] A. Bazavov *et al.*, *Rev. Mod. Phys.* **82**, 1349 (2010), [arXiv:0903.3598 \[hep-lat\]](#)
 - [29] G. C. Donald, C. T. H. Davies, E. Follana, and A. S. Kronfeld, *Phys. Rev.* **D84**, 054501 (2011), [arXiv:1106.2412 \[hep-lat\]](#)
 - [30] J. Laiho, E. Lunghi, and R. S. Van de Water, *Phys. Rev.* **D81**, 034503 (2010), [arXiv:0910.2928 \[hep-ph\]](#)
 - [31] C. W. Bernard *et al.*, *Phys. Rev.* **D64**, 054506 (2001), [arXiv:hep-lat/0104002](#)
 - [32] B. Sheikholeslami and R. Wohlert, *Nucl. Phys.* **B259**, 572 (1985)

- [33] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, [Phys. Rev. D**55**, 3933 \(1997\)](#), [arXiv:hep-lat/9604004](#)
- [34] K. Symanzik, [Nucl. Phys. B**226**, 187 \(1983\)](#)
- [35] K. Symanzik, [Nucl. Phys. B**226**, 205 \(1983\)](#)
- [36] A. S. Kronfeld, [Phys. Rev. D**62**, 014505 \(2000\)](#), [arXiv:hep-lat/0002008](#)
- [37] J. Harada *et al.*, [Phys. Rev. D**65**, 094513 \(2002\)](#), [Erratum-ibid. **D71**, 019903 (2005)], [arXiv:hep-lat/0112044](#)
- [38] J. Harada *et al.*, [Phys. Rev. D**65**, 094514 \(2002\)](#), [arXiv:hep-lat/0112045](#)
- [39] C. Aubin and C. Bernard, [Phys. Rev. D**73**, 014515 \(2006\)](#), [arXiv:hep-lat/0510088](#)
- [40] J. Laiho and R. S. Van de Water, [Phys. Rev. D**73**, 054501 \(2006\)](#), [arXiv:hep-lat/0512007](#)
- [41] C. Aubin and C. Bernard, [Phys. Rev. D**76**, 014002 \(2007\)](#), [arXiv:0704.0795 \[hep-lat\]](#)
- [42] A. X. El-Khadra, A. S. Kronfeld, P. B. Mackenzie, S. M. Ryan, and J. N. Simone, [Phys. Rev. D**64**, 014502 \(2001\)](#), [arXiv:hep-ph/0101023](#)
- [43] A. X. El-Khadra, E. Gámiz, A. S. Kronfeld, and M. A. Nobes, PoS **LAT2007**, 242 (2007), [arXiv:0710.1437 \[hep-lat\]](#)
- [44] C. Aubin *et al.* (Fermilab Lattice and MILC), [Phys. Rev. Lett. **95**, 122002 \(2005\)](#), [arXiv:hep-lat/0506030](#)
- [45] C. Bernard *et al.* (Fermilab Lattice and MILC), PoS **LAT2006**, 094 (2006)
- [46] C. Bernard *et al.* (Fermilab Lattice and MILC), PoS **LAT2007**, 370 (2007)
- [47] C. Bernard *et al.* (Fermilab Lattice and MILC), PoS **LATTICE2008**, 278 (2008), [arXiv:0904.1895 \[hep-lat\]](#)
- [48] A. Bazavov *et al.* (Fermilab Lattice and MILC), PoS **LAT2009**, 249 (2009), [arXiv:0912.5221 \[hep-lat\]](#)
- [49] J. Simone *et al.* (Fermilab Lattice and MILC), PoS **LATTICE2010**, 317 (2010)
- [50] J. L. Rosner and S. Stone(2010), in Ref. [51], [arXiv:1002.1655 \[hep-ex\]](#)
- [51] K. Nakamura *et al.* (Particle Data Group), [J. Phys. G**37**, 075021 \(2010\)](#), and 2011 partial update for the 2012 edition
- [52] C. Aubin *et al.* (Fermilab Lattice and MILC), [Phys. Rev. Lett. **94**, 011601 \(2005\)](#), [arXiv:hep-ph/0408306](#)
- [53] C. Bernard *et al.* (Fermilab Lattice and MILC), [Phys. Rev. D**79**, 014506 \(2009\)](#), [arXiv:0808.2519 \[hep-lat\]](#)
- [54] J. A. Bailey *et al.* (Fermilab Lattice and MILC), [Phys. Rev. D**79**, 054507 \(2009\)](#), [arXiv:0811.3640 \[hep-lat\]](#)
- [55] C. Bernard *et al.* (Fermilab Lattice and MILC), [Phys. Rev. D**83**, 034503 \(2011\)](#), [arXiv:1003.1937 \[hep-lat\]](#)
- [56] G. P. Lepage, [Phys. Rev. D**59**, 074502 \(1999\)](#), [arXiv:hep-lat/9809157](#)
- [57] M. Lüscher and P. Weisz, [Phys. Lett. B**158**, 250 \(1985\)](#)
- [58] Z. Hao, G. M. von Hippel, R. R. Horgan, Q. J. Mason, and H. D. Trottier, [Phys. Rev. D**76**, 034507 \(2007\)](#), [arXiv:0705.4660 \[hep-lat\]](#)
- [59] K. G. Wilson, “Quarks and Strings on a Lattice,” in *New Phenomena In Subnuclear Physics*, edited by A. Zichichi (Plenum, New York, 1975) p. 69, cLNS-321
- [60] M. B. Oktay and A. S. Kronfeld, [Phys. Rev. D**78**, 014504 \(2008\)](#), [arXiv:0803.0523 \[hep-lat\]](#)
- [61] H.-W. Lin and N. Christ, [Phys. Rev. D**76**, 074506 \(2007\)](#), [arXiv:hep-lat/0608005](#)
- [62] G. P. Lepage, L. Magnea, C. Nakhleh, U. Magnea, and K. Hornbostel, [Phys. Rev. D**46**, 4052 \(1992\)](#), [arXiv:hep-lat/9205007](#)
- [63] R. Sommer, [Nucl. Phys. B**411**, 839 \(1994\)](#), [arXiv:hep-lat/9310022](#)

- [64] C. W. Bernard *et al.*, [Phys. Rev. D](#) **D62**, 034503 (2000), [arXiv:hep-lat/0002028](#)
- [65] C. R. Allton(1996), [hep-lat/9610016](#)
- [66] A. Bazavov *et al.* (MILC), PoS **CD09**, 007 (2009), [arXiv:0910.2966 \[hep-ph\]](#)
- [67] C. T. H. Davies, E. Follana, I. D. Kendall, G. P. Lepage, and C. McNeile (HPQCD), [Phys. Rev. D](#) **D81**, 034506 (2010), [arXiv:0910.1229 \[hep-lat\]](#)
- [68] G. P. Lepage *et al.*, [Nucl. Phys. Proc. Suppl.](#) **106**, 12 (2002), [arXiv:hep-lat/0110175](#)
- [69] C. Morningstar, [Nucl. Phys. Proc. Suppl.](#) **109A**, 185 (2002), [arXiv:hep-lat/0112023](#)
- [70] A. S. Kronfeld, [Nucl. Phys. Proc. Suppl.](#) **53**, 401 (1997), [arXiv:hep-lat/9608139](#)
- [71] N. Kawamoto and J. Smit, [Nucl. Phys.](#) **B192**, 100 (1981)
- [72] J. L. Richardson, [Phys. Lett.](#) **B82**, 272 (1979)
- [73] D. P. Menscher, “Charmonium and Charmed Mesons with Improved Lattice QCD,” (2005), PhD thesis
- [74] M. Wingate, J. Shigemitsu, C. T. H. Davies, G. P. Lepage, and H. D. Trottier, [Phys. Rev. D](#) **D67**, 054505 (2003), [arXiv:hep-lat/0211014](#)
- [75] M. D. Pierro and E. Eichten, [Phys. Rev. D](#) **D64**, 114004 (2001), [hep-ph/0104208](#), <http://arxiv.org/abs/hep-ph/0104208>
- [76] G. P. Lepage and P. B. Mackenzie, [Phys. Rev. D](#) **D48**, 2250 (1993), [arXiv:hep-lat/9209022](#)
- [77] Q. Mason *et al.* (HPQCD), [Phys. Rev. Lett.](#) **95**, 052002 (2005), [arXiv:hep-lat/0503005](#)
- [78] K. Hornbostel, G. P. Lepage, and C. Morningstar, [Phys. Rev. D](#) **D67**, 034023 (2003), [arXiv:hep-ph/0208224](#)
- [79] D. Arndt and C. J. D. Lin, [Phys. Rev. D](#) **D70**, 014503 (2004), [arXiv:hep-lat/0403012](#)
- [80] C. Bernard (MILC), [Phys. Rev. D](#) **D65**, 054031 (2002), [arXiv:hep-lat/0111051](#)
- [81] A. S. Kronfeld and S. M. Ryan, [Phys. Lett. B](#) **B543**, 59 (2002), [arXiv:hep-ph/0206058](#)
- [82] C. G. Boyd and B. Grinstein, [Nucl. Phys. B](#) **B442**, 205 (1995), [arXiv:hep-ph/9402340](#)
- [83] I. W. Stewart, [Nucl. Phys. B](#) **B529**, 62 (1998), [arXiv:hep-ph/9803227](#)
- [84] D. Bećirević, S. Prelovšek, and J. Zupan, [Phys. Rev. D](#) **D68**, 074003 (2003), [arXiv:hep-lat/0305001](#)
- [85] C. Bernard *et al.* (MILC), PoS **LATTICE2007**, 090 (2007), [arXiv:0710.1118 \[hep-lat\]](#)
- [86] R. Casalbuoni *et al.*, [Phys. Rept.](#) **281**, 145 (1997), [arXiv:hep-ph/9605342 \[hep-ph\]](#)
- [87] A. Anastassov *et al.* (CLEO), [Phys. Rev. D](#) **D65**, 032003 (2002), [arXiv:hep-ex/0108043](#)
- [88] A. Abada *et al.*, [Nucl. Phys. Proc. Suppl.](#) **119**, 641 (2003), [arXiv:hep-lat/0209092](#)
- [89] M. C. Arnesen, B. Grinstein, I. Z. Rothstein, and I. W. Stewart, [Phys. Rev. Lett.](#) **95**, 071802 (2005), [arXiv:hep-ph/0504209](#)
- [90] H. Ohki, H. Matsufuru, and T. Onogi, [Phys. Rev. D](#) **D77**, 094509 (2008), [arXiv:0802.1563 \[hep-lat\]](#)
- [91] J. Bulava, M. A. Donnellan, and R. Sommer (ALPHA), PoS **LATTICE2010**, 303 (2010), [arXiv:1011.4393 \[hep-lat\]](#)
- [92] C. Aubin *et al.* (HPQCD), [Phys. Rev. D](#) **D70**, 031504 (2004), [arXiv:hep-lat/0405022](#)
- [93] C. Bernard *et al.* (MILC), [Phys. Rev. D](#) **D66**, 094501 (2002), [arXiv:hep-lat/0206016](#)
- [94] G. P. Lepage, in *From actions to answers. Proceedings, Theoretical Advanced Study Institute in Elementary Particle Physics, Boulder, USA, June 5-30, 1989*, edited by T. A. DeGrand and D. Toussaint (World Scientific, 1989)
- [95] C. T. H. Davies, C. McNeile, E. Follana, G. P. Lepage, H. Na, *et al.* (HPQCD), [Phys. Rev. D](#) **D82**, 114504 (2010), [arXiv:1008.4018 \[hep-lat\]](#)
- [96] P. Dimopoulos *et al.* (ETM)(2011), [arXiv:1107.1441 \[hep-lat\]](#)
- [97] B. I. Eisenstein *et al.* (CLEO), [Phys. Rev. D](#) **D78**, 052003 (2008), [arXiv:0806.2112 \[hep-ex\]](#)

- [98] J. P. Alexander *et al.* (CLEO), *Phys. Rev.* **D79**, 052001 (2009), [arXiv:0901.1216 \[hep-ex\]](#)
- [99] L. Widhalm *et al.* (Belle), *Phys. Rev. Lett.* **100**, 241801 (2008), [arXiv:0709.1340 \[hep-ex\]](#)
- [100] P. Naik *et al.* (CLEO), *Phys. Rev.* **D80**, 112004 (2009), [arXiv:0910.3602 \[hep-ex\]](#)
- [101] P. U. E. Onyisi *et al.* (CLEO), *Phys. Rev.* **D79**, 052002 (2009), [arXiv:0901.1147 \[hep-ex\]](#)
- [102] J. P. Lees *et al.* (BaBar), *Phys. Rev.* **D82**, 091103 (2010), [arXiv:1003.3063 \[hep-ex\]](#)
- [103] D. Asner *et al.* (Heavy Flavor Averaging Group)(2010), http://www.slac.stanford.edu/xorg/hfag/charm/CHARM10/f_ds/results_20jan11.html with future updates at <http://www.slac.stanford.edu/xorg/hfag/charm/>, [arXiv:1010.1589 \[hep-ex\]](#)
- [104] C. McNeile, C. T. H. Davies, E. Follana, K. Hornbostel, and G. P. Lepage (HPQCD)(2011), [arXiv:1110.4510 \[hep-lat\]](#)
- [105] E. Gámiz, C. T. H. Davies, G. P. Lepage, J. Shigemitsu, and M. Wingate (HPQCD), *Phys. Rev.* **D80**, 014503 (2009), [arXiv:0902.1815 \[hep-lat\]](#)
- [106] C. Albertus *et al.* (RBC and UKQCD), *Phys. Rev.* **D82**, 014505 (2010), [arXiv:1001.2023 \[hep-lat\]](#)
- [107] A. Bazavov *et al.* (MILC), PoS **LATTICE2010**, 320 (2010), [arXiv:1012.1265 \[hep-lat\]](#)
- [108] E. Follana, C. T. H. Davies, G. P. Lepage, and J. Shigemitsu (HPQCD), *Phys. Rev. Lett.* **100**, 062002 (2008), [arXiv:0706.1726 \[hep-lat\]](#)
- [109] B. P. G. Mertens, A. S. Kronfeld, and A. X. El-Khadra, *Phys. Rev.* **D58**, 034505 (1998), [arXiv:hep-lat/9712024](#)

B and D meson decay constants from 2+1 flavor improved staggered simulations

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We give an update on simulation results for the decay constants f_B, f_{B_s}, f_D and f_{D_s} . These decay constants are important for precision tests of the standard model, in particular entering as inputs to the global CKM unitarity triangle fit. The results presented here make use of the MILC (2+1)-flavor asqtad ensembles, with heavy quarks incorporated using the clover action with the Fermilab method. Partially quenched, staggered chiral perturbation theory is used to extract the decay constants at the physical point. In addition, we give error projections for a new analysis in progress, based on an extended data set.

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1. Introduction

Within the standard model, the decay of mesons containing heavy quarks (in particular, B and D mesons) into purely leptonic final states provides an important testing ground for a number of theoretical ideas. Such decays involve both weak and strong interactions simultaneously, so that a complete understanding of the standard model is necessary to describe them. In particular, the decay width of a charged meson is proportional to both the meson decay constant (determined by strong interactions) and the CKM mixing angle,

$$\Gamma(H \rightarrow \ell \nu_\ell) \propto f_H^2 |V_{Qq}|^2. \quad (1.1)$$

Because this fully leptonic decay has no hadrons in the final state, the meson decay constant f_P can be readily and accurately determined by lattice simulations [1, 2, 3, 4]. Such a determination is in fact necessary in order to extract the CKM angles from experimental measurements of these decays, and precise computations of the decay constants could potentially reveal the presence of new physics through tension in the CKM unitarity triangle [5, 6, 7, 8]. In addition, certain leptonic decay channels (e.g. $B_s \rightarrow \mu^+ \mu^-$) are both loop and CKM suppressed in the standard model, and so they may be particularly sensitive to flavor-changing interactions induced by new physics [9].

2. Simulation Details

We make use of the MILC asqtad-improved staggered gauge configurations, with $2 + 1$ dynamical quarks in the sea [10]. For the light valence quarks, we make use of the same staggered action, while charm and bottom valence quarks are incorporated using the clover action with the Fermilab interpretation [11]. The particular set of ensembles used to obtain the results presented here, along with the number of configurations and other relevant information, are detailed in Table 1. Data on the coarsest lattice spacing $a \approx 0.15$ fm are shown in the analysis but are used only for the purpose of estimating the discretization errors; these points are excluded from the final fit used for chiral and continuum extrapolation.

3. Analysis and Fitting

The heavy meson decay constant is determined through the overlap of the meson wavefunction $|H\rangle$ with the axial vector current:

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle (M_H)^{-1/2} = i(p^\mu / M_H) (f_H \sqrt{M_H}) \equiv i(p^\mu / M_H) \phi_H. \quad (3.1)$$

The quantity $\phi_H \equiv f_H \sqrt{M_H}$ is thus proportional to the ground-state amplitude of the two-point function between the axial vector current and a heavy-light pseudoscalar operator $\mathcal{O}$. We therefore extract ϕ_H by fitting this two-point function simultaneously with the two-point pseudoscalar correlator,

$$\Phi_2^s(t) = \frac{1}{4} \sum_{a=1}^4 \langle A_a^{4\dagger}(t, \mathbf{x}) \mathcal{O}_a^{(s)}(0) \rangle, \quad (3.2)$$

$$C_2^{s,s'}(t) = \frac{1}{4} \sum_{a=1}^4 \langle \mathcal{O}_a^{(s)\dagger}(t, \mathbf{x}) \mathcal{O}_a^{(s')}(0) \rangle, \quad (3.3)$$

$\approx a$ [fm]	am_h	am_l	β	r_1/a	N_{conf}
0.09	0.031	0.0031	7.08	3.75	435
		0.0062	7.09	3.79	557
		0.0124	7.11	3.86	518
0.12	0.050	0.005	6.76	2.74	678
		0.007	6.76	2.74	833
		0.010	6.76	2.74	592
		0.020	6.79	2.82	460
		0.030	6.81	2.88	549
<i>0.15</i>	<i>0.0484</i>	<i>0.0097</i>	<i>6.572</i>	<i>2.22</i>	<i>631</i>
		<i>0.0194</i>	<i>6.586</i>	<i>2.26</i>	<i>631</i>
		<i>0.0290</i>	<i>6.600</i>	<i>2.29</i>	<i>576</i>

Table 1: Table of gauge configurations used for the full analysis to be presented. The ensembles with $a \approx 0.15$ fm (italics) are excluded from the final chiral/continuum extrapolation, as described in the text.

where a is a staggered taste index. Precise definitions of the interpolating operators A^4 and $\mathcal{O}$ are given in Ref. [12].

For a correlation function with source type s and sink type s' , we fit to the “factorized” functional form

$$C_{ss'}(t) = \sum_{n=0}^{N_X} \left[A_{s,n} A_{s',n} \left(e^{-E_n t} + e^{-E_n(N_t-t)} \right) - (-1)^t A'_{s,n} A'_{s',n} \left(e^{-E'_n t} + e^{-E'_n(N_t-t)} \right) \right] \quad (3.4)$$

where N_X denotes the number of excited states included in the fit. The pseudoscalar source and sink type s, s' can be either point-like or smeared, so that a total of six distinct correlators are available for analysis. In the results shown here, joint fits are carried out to various combinations of correlators, with Bayesian priors imposed as constraints on the fit parameters.

From the two-point fits, we extract a bare value for the ground-state amplitude between an axial-vector current and pseudoscalar operator, which must then be renormalized in order to obtain the decay constant:

$$\phi_H = \sqrt{2} Z_{A_{Qq}^4} A_{A_{Qq}^4,0}. \quad (3.5)$$

To compute the heavy-light axial current renormalization constant $Z_{A_{Qq}^4}$, we divide it into flavor-diagonal contributions $Z_{V_{qq}^4}, Z_{V_{QQ}^4}$, which are determined non-perturbatively, and a flavor off-diagonal piece $\rho_{A_{Qq}^4}$ which is computed in lattice perturbation theory [13]. Our renormalized result for $\phi_H = f_H \sqrt{M_H}$ is thus given by

$$\phi_H = \sqrt{2} Z_{A_{Qq}^4} A_{A_{Qq}^4,0} = \sqrt{2} (\rho_{A_{Qq}^4} \sqrt{Z_{V_{qq}^4} Z_{V_{QQ}^4}}) A_{A_{Qq}^4,0}. \quad (3.6)$$

We use rooted staggered chiral perturbation theory (rS χ PT) [14] to extrapolate our results simultaneously to the continuum limit and to the physical light-quark masses. (Heavy quark masses are tuned non-perturbatively to give physical heavy-light meson masses, so no extrapolation is necessary for them. Details of the tuning procedure are given in [15].) The chiral fit functions incorporate terms describing a number of different effects, including discretization errors, finite-volume corrections, and hyperfine splittings.

Table 2: Error budget for the decay constants, as obtained in Section 4. In addition, projected improvements to the decay constant error budget for the updated analysis in progress (discussed in Section 5) are shown italicized and in brackets.

Source	f_{D^+} (MeV)	f_{D_s} (MeV)	f_{B^+} (MeV)	f_{B_s} (MeV)
Statistics	2.3 [1.1]	2.3 [1.1]	3.6 [1.8]	3.4 [1.7]
Heavy-quark disc.	8.2 [3.6]	8.3 [3.6]	3.7 [1.9]	3.8 [2.0]
Light-quark disc.	2.9 [0.7]	1.5 [0.3]	2.5 [0.6]	2.1 [0.5]
Chiral extrapolation	3.2 [1.6]	2.2 [1.1]	2.9 [1.5]	2.8 [1.4]
Heavy-quark tuning	2.8 [2.0]	2.8 [2.0]	3.9 [2.4]	3.9 [2.4]
$Z_{V_{QQ}^4}$ and $Z_{V_{qq}^4}$	2.8 [1.4]	3.4 [1.7]	2.6 [1.5]	3.1 [1.9]
u_0 adjustment	1.8 [0]	2.0 [0]	2.5 [0]	2.8 [0]
Other sources	3.8 [3.8]	3.0 [3.0]	3.5 [3.5]	4.8 [4.8]
Total [projected] error	11.3 [6.1]	10.8 [5.6]	8.9 [5.5]	9.5 [6.4]

4. Results

Applying the procedure outlined above, we obtain the values for ϕ shown in Figures 1 and 2, renormalized and in units of the standard scale r_1 . The chiral best-fit curve to the points is also shown, both explicitly at each lattice spacing and extrapolated to the continuum limit.

Evaluating the continuum best-fit curves at the physical points, we obtain the following values for the decay constants and their ratios:

$$f_{B^+} = 196.9(8.9) \text{ MeV}, \quad (4.1)$$

$$f_{B_s} = 242.0(9.5) \text{ MeV}, \quad (4.2)$$

$$f_{B_s}/f_{B^+} = 1.229(0.026), \quad (4.3)$$

$$f_{D^+} = 218.9(11.3) \text{ MeV}, \quad (4.4)$$

$$f_{D_s} = 260.1(10.8) \text{ MeV}, \quad (4.5)$$

$$f_{D_s}/f_{D^+} = 1.188(0.025). \quad (4.6)$$

The error bars quoted here include both statistical and systematic sources of error, which are accounted for in a detailed error budget. A summary of the full error budget for the individual decay constants is given in Table 2. We discuss the error budget further in Section 5 below, but a thorough discussion is beyond the scope of this paper. Instead, we refer the reader to Ref. [12], which contains a complete discussion of the systematic error analysis, including the full error budget for the decay-constant ratios.

5. Outlook

A new analysis following the approach outlined above is currently in progress, based on an expanded set of gauge configurations as shown in Table 3. In addition to extending the available simulations to finer lattice spacing and smaller quark mass, the “new” data set includes large increases in statistics for several ensembles.

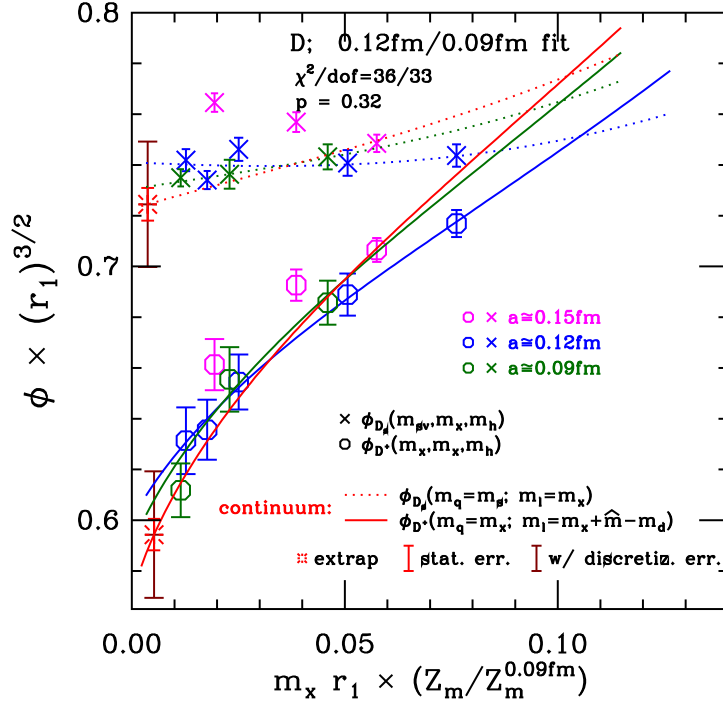


Figure 1: Extracted values of ϕ and chiral best-fit curves for the D system. Only points where valence and sea light-quark masses are equal are shown here. Data from the $a \approx 0.15$ fm ensemble are shown but not included in the fit. The red curve and symbols show the continuum extrapolation and the continuum/physical point extrapolation, respectively, for both ϕ_{D^+} and ϕ_{D_s} . For the fully extrapolated points, the inner error bars (bright red) represent statistical errors only, while the outer errors (dark red) include discretization errors.

Projected improvements in the error budget when the new data set is included are shown alongside the previous error estimates in Table 2. Statistical errors are projected to improve as $\sqrt{N_{\text{cfg}}}$, with N_{cfg} the number of gauge configurations available for a given ensemble. For the various discretization errors, the projected improvements are a result of reducing the smallest lattice spacing available from $a = 0.09$ fm to $a = 0.045$ fm. Light-quark discretization errors are estimated to scale as $\mathcal{O}(\alpha_s a^2)$; the heavy-quark discretization errors are estimated using the known functional dependence, which has several terms. The decrease in the chiral extrapolation error is projected based on the lightest available value of the quark mass in r_1 units, $m_x r_1$. The heavy-quark tuning error is based on a combination of statistical and discretization errors, and is treated as such. The “ u_0 adjustment” error is the result of using different tadpole improvement factors for the valence and sea quarks. This is rectified in the new data analysis, eliminating the associated error. Finally, the error estimates for the heavy-quark renormalization factors $Z_{V_{QQ}^4}, Z_{V_{qq}^4}$ are based on preliminary non-perturbative results for those quantities.

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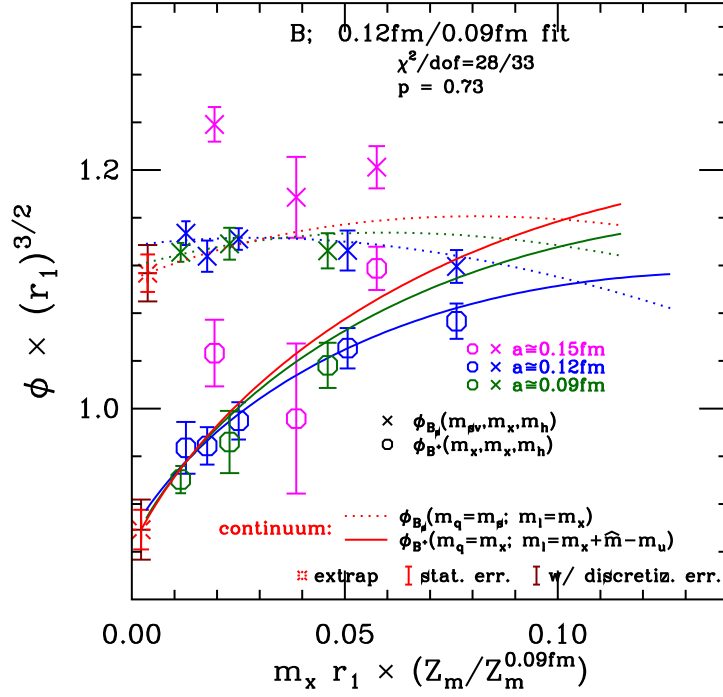


Figure 2: ϕ values and chiral best-fit curves as in Figure 1, but for the B system.

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References

- [1] C. McNeile, C. T. H. Davies, E. Follana, K. Hornbostel and G. P. Lepage, arXiv:1110.4510 [hep-lat].
- [2] C. T. H. Davies *et al.*, Phys. Rev. D **82**, 114504 (2010) [arXiv:1008.4018 [hep-lat]].
- [3] P. Dimopoulos *et al.* [ETM Collaboration], arXiv:1107.1441 [hep-lat].

$\approx a$ [fm]	am_h	am_l	β	r_1/a	N_{conf} (old run)	N_{conf} (new run)
0.045	0.014	0.0028	7.81	7.21	—	800
0.06	0.018	0.0018	7.46	5.31	—	825
		0.0025	7.465	5.33	—	800
		0.0036	7.47	5.35	—	631
		0.0072	7.48	5.40	—	591
		0.00155	7.075	3.74	—	790
0.09	0.031	0.0031	7.08	3.75	435	577
		0.00465	7.085	3.77	—	983
		0.0062	7.09	3.79	557	1377
		0.0124	7.11	3.86	518	1476
		0.005	6.76	2.74	678	1419
0.12	0.050	0.007	6.76	2.74	833	1274
		0.010	6.76	2.74	592	1664
		0.020	6.79	2.82	460	1637
		0.030	6.81	2.88	549	—
		0.0097	6.572	2.22	631	—
0.15	0.0484	0.0194	6.586	2.26	631	—
		0.0290	6.600	2.29	576	—

Table 3: Table of gauge configurations for the updated analysis in progress. Only configurations labelled “old run” were used to obtain the results presented in Section 4. The analysis in progress will make use of all configurations from both runs combined.

- [4] F. Farchioni *et al.*, PoSLATTICE **2010**, 128 (2010) [arXiv:1012.0200 [hep-lat]].
- [5] A. Lenz *et al.* [CKMfitter Collaboration], Phys. Rev. D **83**, 036004 (2011) [arXiv:1008.1593 [hep-ph]].
- [6] E. Lunghi and A. Soni, Phys. Lett. B **697**, 323 (2011) [arXiv:1010.6069 [hep-ph]].
- [7] J. Laiho, E. Lunghi and R. Van De Water, PoSFCP **2010**, 040 (2010) [arXiv:1102.3917 [hep-ph]].
- [8] A. J. Bevan *et al.* [UTfit Collaboration], PoS **ICHEP2010**, 270 (2010) [arXiv:1010.5089 [hep-ph]].
- [9] T. Aaltonen *et al.* [CDF Collaboration], Phys. Rev. Lett. **107**, 191801 (2011) [arXiv:1107.2304 [hep-ex]].
- [10] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010) [arXiv:0903.3598 [hep-lat]].
- [11] A. X. El-Khadra, A. S. Kronfeld and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997) [hep-lat/9604004].
- [12] A. Bazavov *et al.* [Fermilab Lattice and MILC Collaborations], “B- and D-meson decay constants from three-flavor lattice QCD,” [arXiv:1112.3051 [hep-lat]].
- [13] A. X. El-Khadra *et al.*, PoSLAT **2007**, 242 (2007) [arXiv:0710.1437 [hep-lat]].
- [14] C. Aubin and C. Bernard, Phys. Rev. D **73**, 014515 (2006) [hep-lat/0510088].
- [15] C. Bernard *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. D **83**, 034503 (2011) [arXiv:1003.1937 [hep-lat]].

Neutral B mixing from $2 + 1$ flavor lattice QCD: the Standard Model and beyond

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We report on the status of our lattice-QCD calculation of the hadronic contribution to B_d^0 and B_s^0 mixing, with $2 + 1$ flavors of dynamical sea quarks. Preliminary results for hadronic mixing matrix elements are given for a basis of five four-quark, dimension-six, $\Delta B = 2$ mixing operators that spans the space of all possible hadronic mixing contributions in the Standard Model and beyond. At the intermediate stage of analysis reported on in this work, our errors are competitive with published Standard Model matrix element results. For beyond the Standard Model matrix elements, this is the first unquenched calculation and the first new lattice-QCD calculation in ten years.

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1. Introduction

The main goal of particle physics today is the search for new physics. A primary focus of that search is the precision determination of the Cabibbo-Kobayashi-Maskawa (CKM) matrix elements or, more accurately, an overdetermination. To achieve this, many flavor-changing processes are studied by both experiment and theory and the results are combined to look for inconsistencies, which could indicate new physics at work [1, 2, 3]. At the same time, as hints of new physics appear, beyond the Standard Model phenomenologists use the information to constrain, support, or rule out new models [4, 5, 6]. In both cases, lattice-QCD calculations of hadronic matrix elements are crucial.

Neutral B mixing is a promising place to look for new physics for two reasons. First, in the Standard Model it occurs via a loop process in which the contributions are suppressed both by CKM matrix elements, and, for all but the top quark, masses of the loop quark. So, any new physics could present a relatively large signal. Second, many recent reviews of the persistent $2\text{--}3\sigma$ tension between the Standard Model and flavor physics experiments indicate that new physics in B mixing is a likely explanation [1, 2, 3, 4, 5].

The most general $\Delta B = 2$ effective hamiltonian contains eight dimension-six operators

$$\mathcal{H}_{\text{eff}} = \sum_{i=1}^5 C_i \mathcal{O}_i + \sum_{i=1}^3 \tilde{C}_i \tilde{\mathcal{O}}_i, \quad (1.1)$$

with

$$\begin{aligned} \mathcal{O}_1 &= (\bar{b}^\alpha \gamma_\mu L q^\alpha) (\bar{b}^\beta \gamma_\mu L q^\beta), \quad \mathcal{O}_4 = (\bar{b}^\alpha L q^\alpha) (\bar{b}^\beta R q^\beta), \\ \mathcal{O}_2 &= (\bar{b}^\alpha L q^\alpha) (\bar{b}^\beta L q^\beta), \quad \mathcal{O}_5 = (\bar{b}^\alpha L q^\beta) (\bar{b}^\beta R q^\alpha), \\ \mathcal{O}_3 &= (\bar{b}^\alpha L q^\beta) (\bar{b}^\beta L q^\alpha), \end{aligned} \quad (1.2)$$

where α and β are color indices, L and R are the projection operators $\frac{1}{2}(1 \pm \gamma_5)$, and $\tilde{\mathcal{O}}_{1,2,3}$ are obtained from $\mathcal{O}_{1,2,3}$ by $L \rightarrow R$.

Parity conservation of QCD ensures the matrix elements for $\tilde{\mathcal{O}}_{1,2,3}$ are physically equivalent to those for $\mathcal{O}_{1,2,3}$, leaving five independent matrix elements. The matrix element $\langle B_q^0 | \mathcal{O}_1 | \bar{B}_q^0 \rangle$ appears in the Standard Model expression for the B meson mass difference ΔM_q . The matrix element $\langle B_q^0 | \mathcal{O}_2 | \bar{B}_q^0 \rangle$ is needed for renormalization of $\langle B_q^0 | \mathcal{O}_1 | \bar{B}_q^0 \rangle$, and all three can be useful in studies of the width difference $\Delta\Gamma$ and its constraints on new physics [7, 8]. The matrix elements $\langle B_q^0 | \mathcal{O}_4 | \bar{B}_q^0 \rangle$ and $\langle B_q^0 | \mathcal{O}_5 | \bar{B}_q^0 \rangle$ are needed for generic extensions beyond the Standard Model (some examples are given in Refs. [6]).

In the Standard Model,

$$\Delta M_q = \left(\frac{G_F^2 M_W^2 S_0}{4\pi^2 M_{B_q}} \right) \eta_B(\mu) |V_{tb} V_{tq}^*|^2 \langle B_q^0 | \mathcal{O}_1 | \bar{B}_q^0 \rangle(\mu), \quad (1.3)$$

where the quantities in parentheses and η_B are known factors, V_{ij} is a CKM matrix element, and we use relativistic normalization for the states. Measurements of ΔM_q have sub-percent errors [9, 10], so our ability to constrain the CKM matrix contribution $|V_{tb} V_{tq}^*|$ is limited by how precisely we know $\langle B_q^0 | \mathcal{O}_1 | \bar{B}_q^0 \rangle$. Current, published lattice-QCD calculations [11] report errors of just under 14% on $\langle B_q^0 | \mathcal{O}_1 | \bar{B}_q^0 \rangle$.

For B_s mixing only, an unquenched calculation of $\langle B_q^0 | \mathcal{O}_{1,2,3} | \bar{B}_q^0 \rangle$ appeared in Ref. [12], though it includes data at only one lattice spacing, $a \approx 0.12$ fm. The only calculation to date of $\langle B_q^0 | \mathcal{O}_4 | \bar{B}_q^0 \rangle$ and $\langle B_q^0 | \mathcal{O}_5 | \bar{B}_q^0 \rangle$ appeared a decade ago [13]. In that work all five matrix elements were calculated using the quenched approximation for the sea, static heavy valence quarks with an interpolation to m_b , and a linear extrapolation in the light valence mass to reach B_d . These approximations are no longer required in modern lattice-QCD calculations. We include three sea quarks to simulate up, down, and strange; work directly at m_b ; include data at two or more lattice spacings; and use rooted, staggered chiral perturbation theory to guide a simultaneous chiral-continuum extrapolation. This work presents the first full error budget for the beyond the Standard Model matrix elements.

Historically, it has been useful to parametrize the matrix elements as [7, 14]

$$\langle B_q^0 | \mathcal{O}_i | \bar{B}_q^0 \rangle(\mu) = c_i M_{B_q}^2 f_{B_q}^2 B_{B_q}^{(i)}(\mu), \quad (1.4)$$

with coefficients $c_i = (2/3, -5/12, 1/12, 1/2, 1/6)$. The $B_{B_q}^{(i)}$, known as bag parameters, characterize deviation from the so-called vacuum saturation-approximation [15]. Today, it is possible to calculate the $\langle B_q^0 | \mathcal{O}_i | \bar{B}_q^0 \rangle$ without appealing to this approximation and, therefore, without need for introducing the bag parameters. Nevertheless, because of their historical use, at a later stage in this project, we intend to combine results for $\langle B_q^0 | \mathcal{O}_i | \bar{B}_q^0 \rangle$ with our collaboration's results for f_{B_q} to extract the bag parameters in a manner that accounts for correlations between the two calculations. In this work we present preliminary results for the matrix elements and refer the reader to Refs. [16, 17], and references therein, for values of f_{B_q} calculated with similar fermion actions and gauge configurations.

In Sec. 2 we describe details of our calculation. A discussion of the full error budget appears in Sec. 3. In Sec. 4 we report preliminary results, and in Sec. 5 we summarize and discuss the remaining work to be done.

2. Calculation

In this section we review the generation of correlation function data, the extraction of matrix elements from fits to the data, and the renormalization and chiral-continuum extrapolation of the matrix elements.

2.1 Generating Correlation Function Data

Correlation function data are generated using the MILC gauge configurations [18] with $2+1$ flavors of asqtad staggered [19] sea quarks. Bottom valence quarks are simulated using the Fermilab interpretation of the Sheikholeslami-Wohlert (clover) action [20] with hopping parameter κ_b tuned to produce the observed B_s meson mass [21]. Light valence quarks are simulated with the asqtad action. We work in the meson rest frame.

Table 1 lists the ensembles used to date and selected valence quark parameters. For each of the n_{conf} configurations we average over n_{src} sources with temporal spacing $T/4$ and spatial distribution randomized to reduce correlations. At this stage of the calculation, different subsets of data have been analyzed for the different operators. The subsets used are noted in Table 1.

a [fm]	$(\frac{L}{a})^3 \times \frac{T}{a}$	u_0	(am_l, am_h)	am_q	κ_b	$n_{\text{conf}} \times n_{\text{src}}$	$\langle \mathcal{O}_{1,2} \rangle$	$\langle \mathcal{O}_3 \rangle$	$\langle \mathcal{O}_{4,5} \rangle$
0.12	$24^3 \times 64$	0.8678	(0.005, 0.05)	val _{0.12}	0.0901	2099×4	X	X	X
0.12	$20^3 \times 64$	0.8678	(0.007, 0.05)	val _{0.12}	0.0901	2110×4	X	X	X
0.12	$20^3 \times 64$	0.8677	(0.010, 0.05)	val _{0.12}	0.0901	2259×4	X	X	X
0.12	$20^3 \times 64$	0.8688	(0.020, 0.05)	val _{0.12}	0.0918	2052×4	X	X	X
0.09	$40^3 \times 96$	0.8799	(0.0031, 0.031)	val _{0.09}	0.0976	1015×4	X	X	X
0.09	$32^3 \times 96$	0.8781	(0.00465, 0.031)	val _{0.09}	0.0977	984×4	X	X	X
0.09	$28^3 \times 96$	0.8782	(0.0062, 0.031)	val _{0.09}	0.0979	1931×4			X
0.09	$28^3 \times 96$	0.8788	(0.0124, 0.031)	val _{0.09}	0.0982	1996×4			X
0.06	$64^3 \times 144$	0.88764	(0.0018, 0.018)	val _{0.06}	0.1052	828×4	X		

Table 1: Summary of the MILC ensembles and valence masses used in this analysis. Each lattice has an approximate spacing a , spatial extent L , and temporal extent T . The tadpole improvement factor is determined from the expectation value of the average plaquette, $u_0 = \langle \text{plaquette} \rangle^{1/4}$. The light and strange sea-quark masses are m_l and m_h , respectively. The sets of valence masses used, m_q , generally run from $m_h/10$ to m_h , with values given by $\text{val}_{0.12} = \{0.005, 0.007, 0.01, 0.02, 0.03, 0.0349, 0.0415, 0.05\}$, $\text{val}_{0.09} = \{0.0031, 0.0047, 0.0062, 0.0093, 0.0124, 0.0261, 0.031\}$, and $\text{val}_{0.06} = \{0.0018, 0.0025, 0.0036, 0.0054, 0.0072, 0.016, 0.0188\}$. The bottom quark hopping parameter is κ_b . An “X” marks ensembles used in the analysis of each operator.

Data are generated as ensemble average estimates of the vacuum expectation values

$$C^{2\text{pt}}(t) = \sum_{\mathbf{x}} \langle B_q^0(t, \mathbf{x}) B_q^0(0, \mathbf{0})^\dagger \rangle \quad (2.1)$$

and

$$C_i^{3\text{pt}}(t_1, t_2) = \sum_{\mathbf{x}_1, \mathbf{x}_2} \langle B_q^0(t_2, \mathbf{x}_2) \mathcal{O}_i(0, \mathbf{0}) B_q^0(t_1, \mathbf{x}_1) \rangle. \quad (2.2)$$

The B meson creation operator is given by

$$B_q^0(t, \mathbf{x})^\dagger = \sum_{\mathbf{y}} \bar{\psi}(t, \mathbf{y}) S(\mathbf{x}, \mathbf{y}) \gamma_5 q(t, \mathbf{x}), \quad (2.3)$$

and the four-quark mixing operator is

$$\mathcal{O}_i(0, \mathbf{0}) = \bar{\psi}(0, \mathbf{0}) \Gamma_i^{(1)} q(0, \mathbf{0}) \bar{\psi}(0, \mathbf{0}) \Gamma_i^{(2)} q(0, \mathbf{0}). \quad (2.4)$$

Propagators arising from the Wick contraction of naive light-quark fields q are related to staggered quark propagators, generated in our simulation, following Ref. [22]. The heavy-quark field ψ is a four-component Dirac spinor, smeared in the B meson creation operator to improve overlap with the ground state. The smearing function $S(\mathbf{x}, \mathbf{y})$ is based on the quarkonium 1S wavefunction [23]. Heavy-quark fields in the mixing operator are rotated to remove leading order discretization errors [20]. The $\Gamma_i^{(1,2)}$ represent the spin structures appearing in the quark bilinears of Eq. (1.2). The three-point correlation function setup is illustrated in Fig. 1.

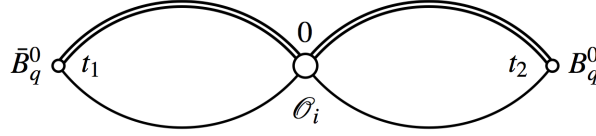


Figure 1: A $\bar{B}_q^0$ is created at rest at $t_1 < 0$. At time 0, via mixing operator $\mathcal{O}_i$, it oscillates into a B_q^0 , which is subsequently annihilated at $t_2 > 0$. The heavy (light) quark propagator is indicated by a double (single) line. To extract the hadronic mixing matrix element we need the three-point correlation function depicted here and the two-point correlation functions corresponding to the propagation of the $\bar{B}_q^0$ from t_1 to 0 and of the B_q^0 from 0 to t_2 .

Although parity conservation of QCD ensures the hadronic mixing matrix elements of $\tilde{\mathcal{O}}_{1,2,3}$ are physically equivalent to those of $\mathcal{O}_{1,2,3}$, the finite statistics estimates of Eq. (2.2) need not generate data that are numerically identical. We average these physically equivalent data to increase statistics associated with the determination of the matrix elements of $\mathcal{O}_{1,2,3}$.

2.2 Fitting Correlation Function Data

We model two- and three-point correlation function data by projecting the vacuum expectation values of Eqs. (2.1) and (2.2) onto bases of B_q^0 and $\bar{B}_q^0$ energy eigenstates,

$$C^{2\text{pt}}(t) = \sum_{n=0}^{N^{2\text{pt}}-1} Z_n^2 (-1)^{n(t+1)} (e^{-E_n t} + e^{-E_n(T-t)}), \quad (2.5)$$

$$C_i^{3\text{pt}}(t_1, t_2) = \sum_{n,m=0}^{N^{3\text{pt}}-1} \frac{Z_n Z_m}{2} \left(\frac{\langle (B_q^0)_n | \mathcal{O}_i | (\bar{B}_q^0)_m \rangle}{\sqrt{E_n E_m}} \right) (-1)^{m(t_1+1)+n(t_2+1)} e^{-E_n t_2} e^{-E_m t_1}, \quad (2.6)$$

where oscillating, opposite-parity state contributions [22] are incorporated. The effects of periodic boundary conditions are negligible in fitted three-point data and are omitted from Eq. (2.6).

We extract the ground state quantity $\langle B_q | \mathcal{O}_i | \bar{B}_q \rangle / M_{B_q}$ by simultaneously fitting the two- and three-point correlation function data to Eqs. (2.5) and (2.6). In principle the sums run over infinitely many radial excitations of the pseudoscalar B meson, in practice we must fit with finite $N^{2,3\text{pt}}$. We also restrict data included in the fit ($t_{\min} \leq t \leq t_{\max}$). Fits using data at short times must account for excited state contributions by including adequate numbers of states. Despite added difficulty, the relatively clean signal in the data at short times makes it desirable to include them in the fit. The use of a Bayesian fitting routine [24, 25] allows us to deal with the difficulty of fitting numerous states and incorporate data at short times. Increasing $t_{\max}$ has the benefit of utilizing more data. However, this also introduces an increasing level of noise and can lead to a poorly determined covariance matrix.

From plots of correlation function data, scaled to remove leading exponential decay, we determine a range of potential $t_{\min}^{2,3\text{pt}}$ and $t_{\max}^{2,3\text{pt}}$ values to study.¹ The range of potential $t_{\max}^{2,3\text{pt}}$ values is determined by the onset of significant noise. For $t_{\min}^{2,3\text{pt}}$ we consider from $t_{\min}^{2,3\text{pt}} = 2$ until excited

¹For $C_i^{3\text{pt}}(t_1, t_2)$, we could choose distinct $t_{1,\min}$ and $t_{2,\min}$ and distinct $t_{1,\max}$ and $t_{2,\max}$. However, an explicit $t_1 \leftrightarrow t_2$ symmetry of data generated by Eq. (2.2) prompts the simplifications: $t_{\min}^{3\text{pt}} \equiv t_{1,\min} = t_{2,\min}$ and $t_{\max}^{3\text{pt}} \equiv t_{1,\max} = t_{2,\max}$.

state contributions have significantly decreased. We perform fits with $N^{2,3\text{pt}} = 2, 4$, and (sometimes) 6.² Starting with the two-point correlation functions, we fit each combination of $N^{2\text{pt}}$, $t_{\min}^{2\text{pt}}$, and $t_{\max}^{2\text{pt}}$ and select representative fits at each $N^{2\text{pt}}$ from a common plateau of fit results for Z_0 and E_0 versus $t_{\min}^{2\text{pt}}$ and $t_{\max}^{2\text{pt}}$, thereby ensuring stability with respect to $N^{2\text{pt}}$, $t_{\min}^{2\text{pt}}$, and $t_{\max}^{2\text{pt}}$. Then, fixing $t_{\min}^{2\text{pt}}$ and $t_{\max}^{2\text{pt}}$ separately for each $N^{2\text{pt}}$, we repeat the procedure for a simultaneous fit of the two- and three-point correlation function data. For these fits, we fix $N^{2\text{pt}} = N^{3\text{pt}}$ and determine the optimum $N^{3\text{pt}}$, $t_{\min}^{3\text{pt}}$, and $t_{\max}^{3\text{pt}}$. This systematic procedure, outlined in more detail in [26, 27], allows us to obtain fit results that are stable in the number of states and data included in the fit. We find the fit results are largely insensitive to changes in $t_{\max}^{2,3\text{pt}}$.

2.3 Renormalization

Lattice results for the hadronic mixing matrix elements are combined with perturbatively calculated Wilson coefficients, *i.e.* C_i and $\tilde{C}_i$ of Eq. (1.1), to obtain physical quantities. Therefore, the lattice and continuum results must be brought to the same scheme and scale. We use the mass of the bottom quark to set the scale and match to the continuum $\overline{\text{MS}}$ –NDR scheme. At one loop the matrix elements mix under renormalization,

$$\langle B | \mathcal{O}_i | \bar{B} \rangle^{\overline{\text{MS}}\text{--NDR}}(m_b) = \sum_{j=1}^5 [\delta_{ij} + \alpha_s(q^*) \zeta_{ij}(am_b)] \langle B | \mathcal{O}_j | \bar{B} \rangle^{\text{lat}}, \quad (2.7)$$

where the matching coefficients ζ_{ij} give the difference between the one-loop lattice and continuum renormalizations [28]. We evaluate $\alpha_s(q^*)$, as in [29], in the “V scheme” [30] at the scale $q^* = 2/a$. $\overline{\text{MS}}$ –NDR is not sufficient to define the matrix elements of operators $\mathcal{O}_2$ and $\mathcal{O}_3$ in dimensional regularization; one must also choose a set of “evanescent” operators. The renormalization coefficients ζ_{2j} and ζ_{3j} must be calculated accordingly. Below, we present results for two schemes, which we label “BBGLN” [31] and “BJU” [32]. The one-loop conversion between the two schemes was first given in Ref. [13]. A more general transformation of the two-loop anomalous dimension matrix can be found in [33]. For convenience, we define the shorthand $\langle \mathcal{O}_i \rangle \equiv \langle B | \mathcal{O}_i | \bar{B} \rangle^{\overline{\text{MS}}\text{--NDR}}(m_b)$, for the matrix elements after extrapolating the renormalized results to the continuum.

2.4 Chiral-Continuum Extrapolation

The continuum, next-to-leading order (NLO), chiral perturbation theory for hadronic mixing matrix elements [34], modified [35] for the rooted, staggered, light-quark actions (rS χ PT), guides a simultaneous extrapolation to physical quark mass and the continuum. The rS χ PT expression is fit to the renormalized matrix elements of Eq. (2.7) to determine the low energy constants. Effects from heavy-light meson flavor- and hyperfine-splittings [16] and finite volume (expected to be $< 1\%$) are not explicitly incorporated in the chiral extrapolations presented here, but will be in the final stage of analysis. Chiral fits are performed using a Bayesian fitting routine [24, 25] with priors constraining each fit parameter. Additional details will be given in future publications.

A chiral expansion including only NLO terms fits the data reasonably well when data included in the fit are limited to light valence masses (*i.e.*, values of m_q such that the pseudoscalar meson

²We use equal numbers of parity-even and parity-odd states in our fits.

mass of Eq. (2.9) satisfies $(M_{qq} r_1)^2 \lesssim 1$.³ To include data at all simulated valence masses we find it necessary to include NNLO analytic terms. There are seven potential NNLO analytic terms [36]

$$a^2 M_{qq}^2, \quad a^2 (2M_{ll}^2 + M_{hh}^2), \quad M_{qq}^2 (2M_{ll}^2 + M_{hh}^2), \quad M_{qq}^4, \quad (2M_{ll}^2 + M_{hh}^2)^2, \quad a^4, \quad (2M_{ll}^4 + M_{hh}^4), \quad (2.8)$$

where the (squared) pseudoscalar meson mass is given by

$$M_{ij}^2 = B_0(m_i + m_j) \quad (2.9)$$

and B_0 is a low-energy constant from χ PT. Each of these terms comes with a coefficient to be determined by the fit. At a minimum, we find it necessary to include terms proportional to $a^2 M_{qq}^2$ and $M_{qq}^2 (2M_{ll}^2 + M_{hh}^2)$ in order to achieve suitable fits to data at all valence masses.

Reported central values are obtained from those fits including all seven NNLO terms. The simultaneous chiral-continuum extrapolations of $\langle \mathcal{O}_i \rangle / M_B$ are shown in Figs. 2, 3, 4, 5, and 6. The p-values of these fits are very near one. This is not the case for NLO fits or fits including various subsets of the possible NNLO analytic terms of Eq. (2.8). Inflated p-values, at least partially, result from the fact that we use the Bayesian augmented χ^2 and degrees of freedom. In addition, the size of our statistical sample may be limiting our ability to resolve small eigenvalues of the correlation matrix. We are studying this issue.

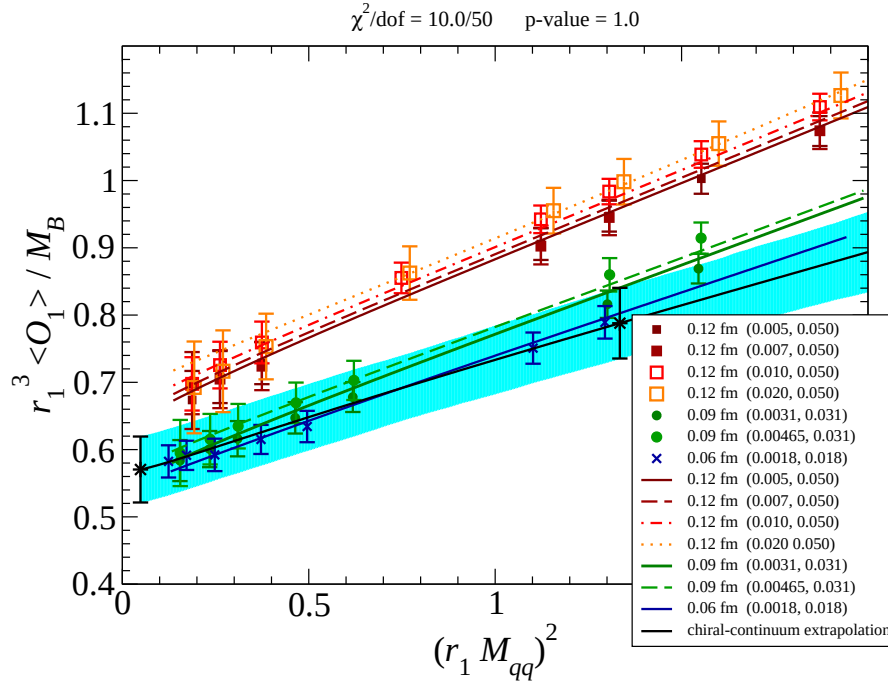


Figure 2: $\langle \mathcal{O}_1 \rangle$: chiral-continuum extrapolation data and fits. (Red/orange) squares are 0.12 fm data, (green) circles are 0.09 fm data, and (blue) $\times$'s are 0.06 fm data. The extrapolation/interpolation is the black line with a shaded (turquoise) error band. Black bursts mark the point of extrapolation (interpolation) for the B_d (B_s) meson.

³For reference, at the strange valence mass, $(M_{qq} r_1)^2 \sim 1.3$.

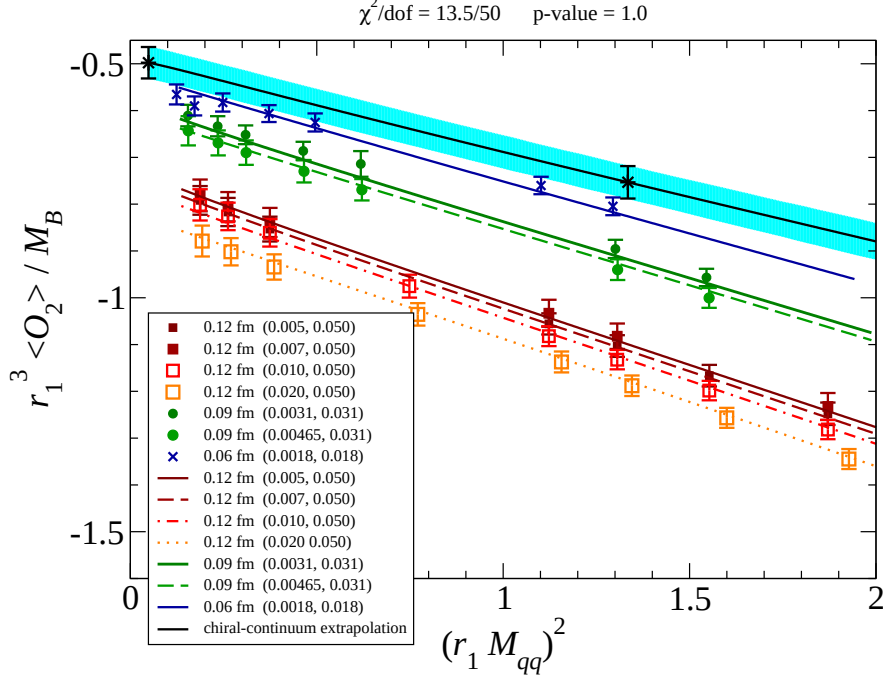


Figure 3: $\langle \mathcal{O}_2 \rangle$: chiral-continuum extrapolation data and fits in the BBGLN scheme described in Sec. 2.3. (Red/orange) squares are 0.12 fm data, (green) circles are 0.09 fm data, and (blue) $\times$'s are 0.06 fm data. The extrapolation/interpolation is the black line with a shaded (turquoise) error band. Black bursts mark the point of extrapolation (interpolation) for the B_d (B_s) meson.

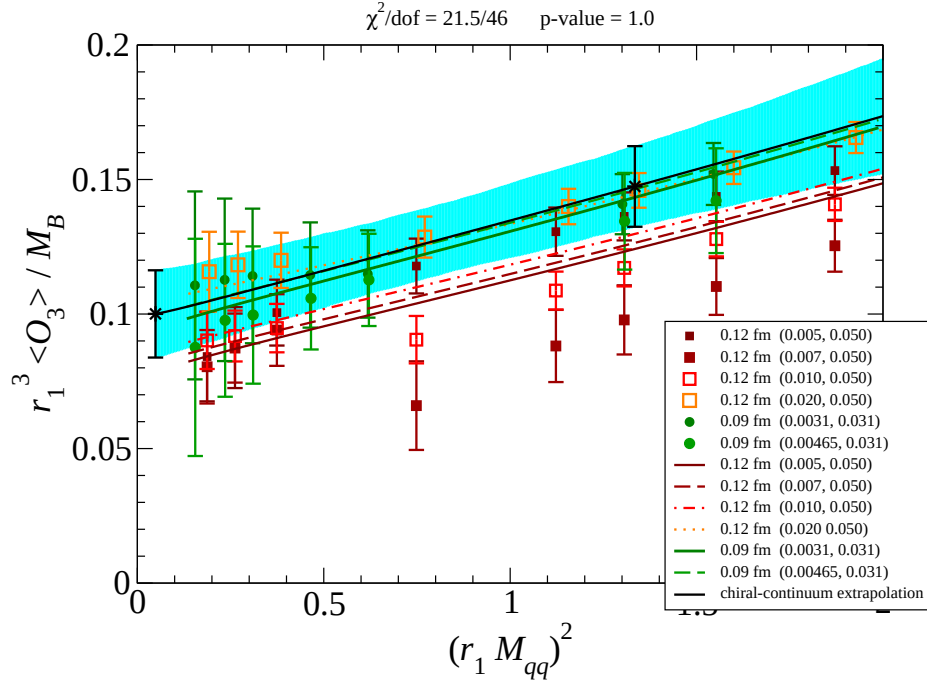


Figure 4: $\langle \mathcal{O}_3 \rangle$: chiral-continuum extrapolation data and fits in the BBGLN scheme described in Sec. 2.3. (Red/orange) squares are 0.12 fm data and (green) circles are 0.09 fm data. The extrapolation/interpolation is the black line with a shaded (turquoise) error band. Black bursts mark the point of extrapolation (interpolation) for the B_d (B_s) meson.

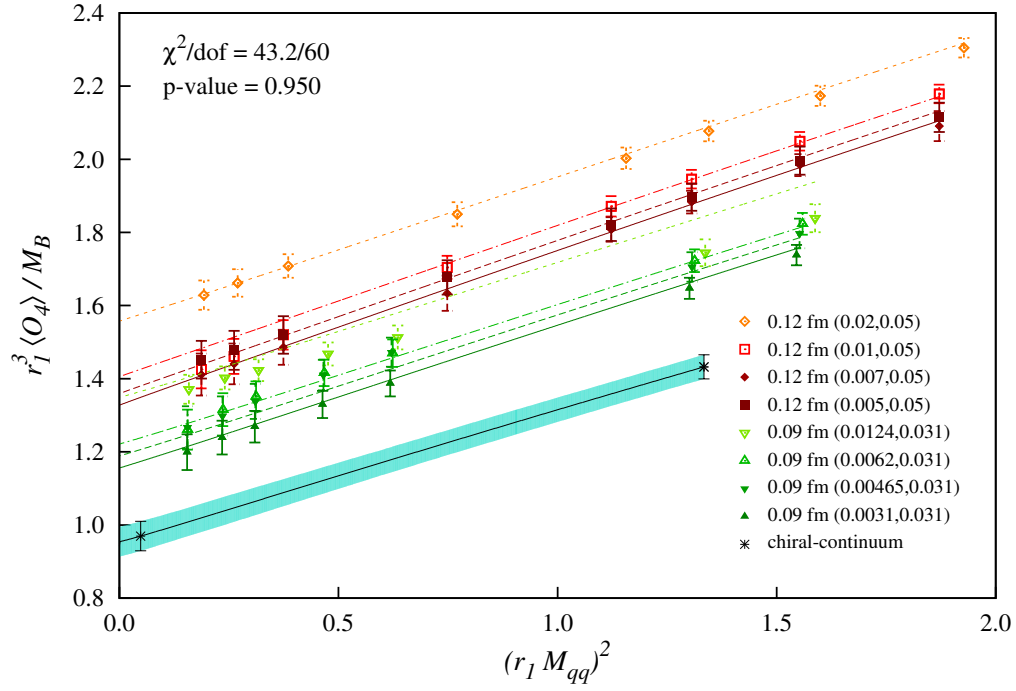


Figure 5: $\langle O_4 \rangle$: chiral-continuum extrapolation data and fits. (Red/orange) squares are 0.12 fm data, (green) triangles are 0.09 fm data. The extrapolation/interpolation is the black line with a shaded (turquoise) error band. Black bursts mark the point of extrapolation (interpolation) for the B_d (B_s) meson.

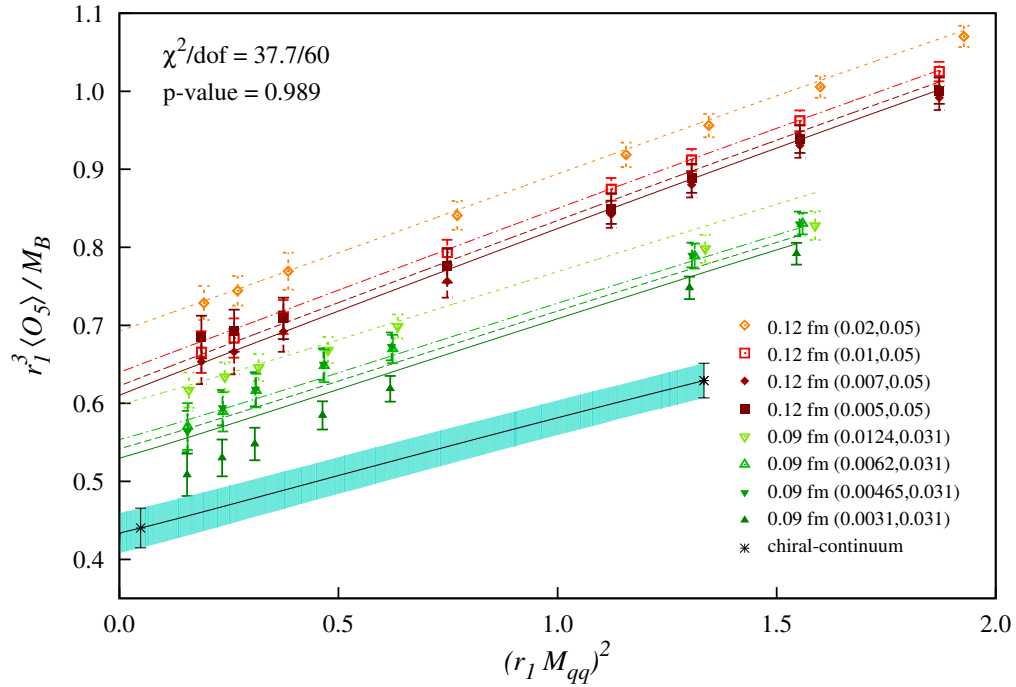


Figure 6: $\langle O_5 \rangle$: chiral-continuum extrapolation data and fits. (Red/orange) squares are 0.12 fm data, (green) triangles are 0.09 fm data. The extrapolation/interpolation is the black line with a shaded (turquoise) error band. Black bursts mark the point of extrapolation (interpolation) for the B_d (B_s) meson.

	Source of Error [%]	$\langle \mathcal{O}_1 \rangle$	$\langle \mathcal{O}_2 \rangle$	$\langle \mathcal{O}_3 \rangle$	$\langle \mathcal{O}_4 \rangle$	$\langle \mathcal{O}_5 \rangle$
B_d^0	statistical	8.6	6.8	16	4.3	5.5
	chiral-continuum systematic	12	11	3.3	0.2	4.4
B_s^0	statistical	6.7	4.6	10	2.5	3.4
	chiral-continuum systematic	1.8	6.6	4.5	1.6	3.7

Table 2: Statistical and chiral-continuum systematic errors for the hadronic mixing matrix elements are determined from the data by methods outlined in Sec. 3. Here we show results from the use of the BBGLN evanescent operators in the renormalization, as described in Sec. 2.3. To the precision reported here, errors in the BJU scheme differ only for the chiral-continuum systematic error for B_s^0 mixing via $\langle \mathcal{O}_2 \rangle$, where we found the error to be 6.4%.

Source of Error [%]	$\langle \mathcal{O}_i \rangle$
scale (r_1)	3
κ_b tuning	4
light-quark masses	1
heavy-quark discretization	4
one-loop matching	8
finite-volume effects	1
subtotal	10

Table 3: Estimates of errors based on our collaboration’s previous works [16, 37]. We anticipate significant reduction in the leading sources of error once all ensembles at $a \approx 0.06$ fm and at $a \approx 0.45$ fm have been fully incorporated into the analysis.

3. Errors

The error budget given in this work is complete in that it accounts for all known, significant sources of error in our lattice-QCD calculation. We have split the list of errors into two tables. Table 2 lists the statistical and chiral-continuum errors, which are determined directly from the analysis presented here, for each $\langle \mathcal{O}_i \rangle$ individually. Errors estimated from our collaboration’s previous works [16, 37] are listed in Table 3 and are taken (for now) to be the same for all $\langle \mathcal{O}_i \rangle$. Errors associated with omitting charm and heavier sea-quark contributions, isospin breaking, and electromagnetic effects are expected to be insignificant in comparison to the errors in Tables 2 and 3. Further study, and an ongoing analysis of $a \approx 0.06$ fm and $a \approx 0.045$ fm data, should lead to a reduction of our leading sources of error in Tables 2 and 3.

Statistical errors are obtained by propagating a distribution of 600 bootstrap ensembles of correlation function data (*i.e.*, Eqs. (2.5 and 2.6)) through the correlation function and rS χ PT fitting procedures, providing non-parametric error estimates that account for correlations among the data. This error also includes uncertainty associated with chiral fit parameters f_π and $g_{B^*B\pi}$ by setting prior widths based on parameter uncertainties.

The systematic error associated with the chiral-continuum series truncation and extrapolation is obtained by varying the rS χ PT fit ansatz. For both the B_d^0 and B_s^0 matrix elements, the addition of the two minimum required NNLO analytic terms of Eq. (2.8) is necessary, and sufficient, to achieve good fits to all valence mass data that are stable against the addition of remaining NNLO terms. We estimate the systematic error to be the shift in fit central values between fits with the two required NNLO analytic terms and those with all NNLO analytic terms.

The remaining errors, quoted in Table 3, are conservative estimates based on previous collaboration publications. The errors associated with scale-setting and κ_b tuning are estimated from Ref. [16]. Entries for light-quark mass, heavy-quark discretization, and one-loop matching errors are estimated from Ref. [37]. Finite volume error estimates are based on Ref. [37] and inflated to accommodate an expected increase [38] from hyperfine- and flavor-splitting effects.

4. Results

Results from our chiral-continuum extrapolations are in r_1 units. We convert to GeV using the lattice determination $r_1 = 0.3117(22)$ fm [16] and the conversion factor $1 \text{ GeV fm} = 5.0677312(1)$. In lieu of the matrix elements, in Table 4 we report the phenomenologically more useful quantity $f_{B_q}^2 B_{B_q}^{(i)}$. Results are given in the continuum $\overline{\text{MS}}$ –NDR scheme at scale m_b using both the BBGLN [31] and BJU [32] choices of evanescent operators. Applying a heavy-quark relation between the matrix elements of $\mathcal{O}_1$, $\mathcal{O}_2$, and $\mathcal{O}_3$, the conversion [13] for bag parameters can be expressed as

$$B_{B_q}^{(2)BJU} = B_{B_q}^{(2)BBGLN} + \frac{\alpha_s}{4\pi} \left(\frac{4}{15} B_{B_q}^{(1)} - 4 B_{B_q}^{(2)} \right), \quad (4.1)$$

$$B_{B_q}^{(3)BJU} = B_{B_q}^{(3)BBGLN} + \frac{\alpha_s}{4\pi} \left(-\frac{4}{3} B_{B_q}^{(1)} + \frac{4}{3} B_{B_q}^{(3)} \right). \quad (4.2)$$

For the results given in Table 4, we bring the matrix elements to the BBGLN or BJU scheme before the chiral-continuum extrapolation. Converting *a posteriori* with Eqs. (4.1) and (4.2) yields values in very good agreement.

The scheme dependence of the $f_{B_q}^2 B_{B_q}^{(i)}$ from Table 4 matches the corresponding scheme dependence in the Wilson coefficients with which they will be used. In particular, one must use the BBGLN or BJU values for $\langle \mathcal{O}_2 \rangle$ and $\langle \mathcal{O}_3 \rangle$, according to the choice of evanescent operator scheme used in the Wilson coefficient calculation. As mentioned in Sec. 2.3, $\langle \mathcal{O}_1 \rangle$, $\langle \mathcal{O}_4 \rangle$, and $\langle \mathcal{O}_5 \rangle$ are independent of this choice.

Errors are obtained by adding in quadrature the appropriate errors from Table 2 and the subtotal of Table 3. As shown in Table 2 and illustrated in Fig. 4, the matrix element $\langle B_q^0 | \mathcal{O}_3 | \bar{B}_q^0 \rangle$ suffers from much larger errors than the others and is more difficult to analyze. We are optimistic that the addition of data at finer lattice spacings, and refinements in analysis techniques, will lead to improvements.

5. Summary and Outlook

We report on our ongoing, $2 + 1$ flavor, lattice-QCD calculation of the hadronic contribution to B^0 and B_s^0 mixing. Table 4 gives preliminary results for the hadronic mixing matrix elements for

[GeV ²]	B_d^0		B_s^0	
	BBGLN	BJU	BBGLN	BJU
$f_{B_q}^2 B_{B_q}^{(1)}$	0.0411(75)		0.0559(68)	
$f_{B_q}^2 B_{B_q}^{(2)}$	0.0574(92)	0.0538(87)	0.086(11)	0.080(10)
$f_{B_q}^2 B_{B_q}^{(3)}$	0.058(11)	0.058(11)	0.084(13)	0.084(13)
$f_{B_q}^2 B_{B_q}^{(4)}$	0.093(10)		0.135(15)	
$f_{B_q}^2 B_{B_q}^{(5)}$	0.127(15)		0.178(20)	

Table 4: Preliminary results for $f_{B_q}^2 B_{B_q}^{(i)} = \langle \mathcal{O}_i \rangle / c_i M_{B_q}^2$, evaluated in the continuum $\overline{\text{MS}}$ –NDR scheme at scale m_b . “BBGLN” and “BJU” denote the choice of evanescent operators in the renormalization schemes of Refs. [31, 32], respectively. For $i = 1, 4, 5$, the schemes are the same. Although the chiral-continuum extrapolation was done separately for both schemes, its output for $f_{B_q}^2 B_{B_q}^{(3)}$ is the same for the number of digits shown. The B_q^0 meson masses, needed in combination with the quantity extracted in Eq. (2.6), are known to $\lesssim 0.01\%$ [10] and do not contribute significantly to the error.

a basis of four-quark, dimension-six, $\Delta B = 2$ mixing operators that spans the space of all possible hadronic contributions in the Standard Model and beyond. At the current stage of analysis our errors are competitive with published Standard Model matrix element results. For beyond the Standard Model matrix elements, this is the first unquenched calculation and the first update in ten years.

Additional data at finer lattice spacings, $a \approx 0.06$ fm and $a \approx 0.045$ fm, is currently being analyzed. We anticipate that its inclusion, and a more rigorous analysis of the errors of Table 3, will result in a significant reduction in the error budget. The discretization and one-loop matching errors of Table 3 are based on $a \approx 0.09$ fm data, and will decrease when re-evaluated for $a \approx 0.045$ fm. Recent data runs will allow for a new analysis of κ_b tuning errors as well. We are finalizing the calculation of the one-loop perturbative matching coefficients of Sec. 2.3 and plan to incorporate finite volume effects and hyperfine- and flavor-splittings in the chiral-continuum extrapolation.

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References

- [1] J. Laiho, E. Lunghi and R.S. Van de Water, Phys. Rev. D **81**, 034503 (2010) [[arXiv:0910.2928](#)].
- [2] E. Lunghi and A. Soni, Phys. Rev. Lett. **104**, 251802 (2010) [[arXiv:0912.0002](#)].
- [3] J. Laiho, E. Lunghi and R.S. Van de Water, PoS **FPCP2010**, 040 (2010) [[arXiv:1102.3917](#)].
- [4] A. Lenz *et al.*, Phys. Rev. D **83**, 036004 (2011) [[arXiv:1008.1593](#)].
- [5] M. Bona *et al.* [UTfit], PMC Phys. A **3**, 6 (2009) [[arXiv:0803.0659](#)].
- [6] W. Altmannshofer and M. Carena, [[arXiv:1110.0843](#)]; M. Bona *et al.* [UTfit], JHEP **0803**, 049 (2008) [[arXiv:0707.0636](#)]; B.A. Dobrescu and G.Z. Krnjaic, [[arXiv:1104.2893](#)].
- [7] A. Lenz and U. Nierste, JHEP **0706**, 072 (2007) [[arXiv:hep-ph/0612167](#)].
- [8] CDF/DØ $\Delta\Gamma_s$, β_s Combination Working Group, CDF Note 9787 and DØ Note 5928, (2009)
- [9] A. Abulencia *et al.* [CDF], Phys. Rev. Lett. **97**, 242003 (2006) [[arXiv:hep-ex/0609040](#)].
- [10] K. Nakamura *et al.* [Particle Data Group], J. Phys. G **37**, 075021 (2010) and 2011 partial update for the 2012 edition [<http://pdg.lbl.gov>].
- [11] E. Gámiz *et al.* [HPQCD], Phys. Rev. D **80**, 014503 (2009) [[arXiv:0902.1815](#)].
- [12] E. Dalgic *et al.*, Phys. Rev. D **76**, 011501 (2007) [[arXiv:hep-lat/0610104](#)]; J. Shigemitsu *et al.* [HPQCD], PoS **Lattice 2006** 093.
- [13] D. Bećirević *et al.*, JHEP **0204**, 025 (2002) [[arXiv:hep-lat/0110091](#)].
- [14] M. Beneke, G. Buchalla and I. Dunietz, Phys. Rev. D **54**, 4419 (1996) [Erratum-ibid. D **83**, 119902 (2011)] [[arXiv:hep-ph/9605259](#)].
- [15] B.W. Lee, J.R. Primack, and S.B. Treiman, Phys. Rev. D **7**, 510 (1973).
- [16] A. Bazavov *et al.*, [Fermilab Lattice and MILC], [arXiv:1112.3051](#).
- [17] E.T. Neil *et al.* [Fermilab Lattice and MILC], PoS **Lattice 2011** 320 [[arXiv:1112.3987](#)].
- [18] A. Bazavov *et al.* [MILC], Rev. Mod. Phys. **82**, 1349 (2010) [[arXiv:0903.3598](#)].
- [19] C. Bernard *et al.* [MILC], Nucl. Phys. (Proc. Suppl.), **60A**, 297 (1998); Phys. Rev. D **58**, 014503 (1998) [[arXiv:hep-lat/9712010](#)]; G.P. Lepage, Nucl. Phys. (Proc. Suppl.), **60A**, 267 (1998) [[arXiv:hep-lat/9707026](#)]; Phys. Rev. D **59**, 074502 (1999) [[arXiv:hep-lat/9809157](#)]; Kostas Orginos and Doug Toussaint [MILC], Nucl. Phys. (Proc. Suppl.), **73**, 909 (1999) [[arXiv:hep-lat/9809148](#)]; Phys. Rev. D **59**, 014501 (1999) [[arXiv:hep-lat/9805009](#)]; Kostas Orginos, Doug Toussaint and R.L. Sugar [MILC], Phys. Rev. D **60**, 054503 (1999) [[arXiv:hep-lat/9903032](#)]; C. Bernard *et al.* [MILC], Phys. Rev. D **61**, 111502 (2000) [[arXiv:hep-lat/9912018](#)].
- [20] A.X. El-Khadra, A.S. Kronfeld, and P.B. Mackenzie, Phys. Rev. D **55**, 3933 (1997) [[arXiv:hep-lat/9604004](#)].

- [21] C. Bernard *et al.* [Fermilab Lattice and MILC], Phys. Rev. D **83**, 034503 (2011) [[arXiv:1003.1937](#)].
- [22] M. Wingate *et al.*, Phys. Rev. D **67**, 054505 (2003) [[arXiv:hep-lat/0211014](#)].
- [23] M. Di Pierro *et al.*, Nucl. Phys. (Proc. Suppl.) **119**, 586 (2002) [[arXiv:hep-lat/0210051](#)].
- [24] G.P. Lepage *et al.*, Nucl. Phys. Proc. Suppl. **106**, 12 (2002) [[arXiv:hep-lat/0110175](#)].
- [25] G.P. Lepage's Python-based library for Bayesian least squares fitting of multi-dimensional, nonlinear functions of arbitrarily many parameters, built around `lsqfit` (2008).
- [26] C.M. Bouchard, Ph.D. thesis, University of Illinois (2011) [[FERMILAB-THESIS-2011-32](#)].
- [27] C.M. Bouchard *et al.* [Fermilab Lattice and MILC], PoS **Lattice 2010** 299 [[arXiv:1011.2570](#)].
- [28] E. Gámiz *et al.* [HPQCD], Phys. Rev. D **77**, 114505 (2008) [[arXiv:0804.1557](#)]; E. Gámiz, A.X. El-Khadra, and A.S. Kronfeld, *in preparation*.
- [29] Q. Mason *et al.*, Phys. Rev. Lett. **95**, 052002 (2005) [[arXiv:hep-lat/0503005](#)].
- [30] G.P. Lepage and P.B. Mackenzie, Phys. Rev. D **48**, 2250 (1993) [[arXiv:hep-lat/9209022](#)].
- [31] M. Beneke *et al.*, Phys. Lett. B **459**, 631 (1999) [[arXiv:hep-ph/9808385](#)].
- [32] A.J. Buras, S. Jager and J. Urban, Nucl. Phys. B **605**, 600 (2001) [[hep-ph/0102316](#)].
- [33] M. Gorbahn, S. Jager, U. Nierste and S. Trine, Phys. Rev. D **84**, 034030 (2011) [[arXiv:0901.2065](#)].
- [34] W. Detmold and C.-J. David Lin, Phys. Rev. D **76**, 014501 (2007) [[arXiv:hep-lat/0612028](#)].
- [35] A. Bazavov *et al.* [Fermilab Lattice and MILC], *in preparation*. Work on Standard Model B mixing using $a \approx 0.09$ fm and coarser lattices.
- [36] R.T. Evans, Ph.D. thesis, University of Illinois (2008) [[www.hep.uiuc.edu/hepg/Theses/Evans_2008.pdf](#)].
- [37] R.T. Evans, *et al.* [Fermilab Lattice and MILC], PoS **Lattice 2009** 245 [[arXiv:0911.5432](#)].
- [38] D. Arndt and C.-J. David Lin Phys. Rev. D **70**, 014503 (2004) [[arXiv:hep-lat/0403012](#)].

Status of the MILC calculation of electromagnetic contributions to pseudoscalar masses

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We calculate pseudoscalar masses on gauge configurations containing the effects of 2+1 flavors of dynamical asqtad quarks and quenched electromagnetism. The lattice spacings vary from 0.12 to 0.06 fm. The masses are fit with staggered chiral perturbation theory including NLO electromagnetic terms. We attempt to extract the fit parameters for the electromagnetic contributions, while taking into account the finite volume effects, and extrapolate them to the physical limit.

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1. Introduction

Quark masses are fundamental parameters in the Standard Model and their determination from lattice field theory is important for phenomenology. With the advance of high-precision spectroscopy the electromagnetic (EM) contributions to the quark masses have become important. In fact, they constitute the largest uncertainty in the calculation of m_u/m_d [1] as indicated in Table 1. The EM error stems from uncertainties in the size of the EM contributions to the masses of the π and especially the K mesons. The contributions have until recently been taken from a variety of phenomenological estimates, and therefore have quite large and not well controlled errors. The MILC collaboration has been working on reducing these uncertainties and progress has been reported previously in Refs. [2, 3, 4].

To lowest order (LO) in chiral perturbation theory (χPT) the electromagnetic splitting in the pion and kaon systems is identical (this observation is known as Dashen’s theorem [5]). We aim to calculate on the lattice the corrections to Dashen’s theorem by employing staggered χPT with EM effects for fits to spectrum data. The corrections to Dashen’s theorem may be parametrized as [6]:

$$(M_{K^\pm}^2 - M_{K^0}^2)^\gamma = (1 + \varepsilon)(M_{\pi^\pm}^2 - M_{\pi^0}^2)^\gamma, \quad (1.1)$$

where the superscript γ denotes the EM contributions.¹ Our main motivation for computing ε is to be able to remove the EM effects from the experimental K masses; the resulting pure-QCD masses may be compared with QCD simulations in order to extract m_u/m_d . Staggered χPT , developed in Ref. [3], gives for the EM splitting between Goldstone pseudoscalars with charged and neutral quarks, $\Delta M_{xy,5}^2$, the following NLO expression:

$$\begin{aligned} \Delta M_{xy,5}^2 = & q_{xy}^2 \delta_{EM} - \frac{1}{16\pi^2} e^2 q_{xy}^2 M_{xy,5}^2 \left[3 \ln(M_{xy,5}^2 / \Lambda_\chi^2) - 4 \right] \\ & - \frac{2\delta_{EM}}{16\pi^2 f^2} \frac{1}{16} \sum_{\sigma, \xi} \left[q_{x\sigma} q_{xy} l(M_{x\sigma, \xi}^2) - q_{y\sigma} q_{xy} l(M_{y\sigma, \xi}^2) \right] + (\text{analytic terms}) \end{aligned} \quad (1.2)$$

where σ is the sea-quark label, ξ is the staggered taste, q_{xy} is the charge of a meson made of a quark x and an antiquark y (for more details on the notations see Ref. [3]). To fit our spectrum data,

	m_u [MeV]	m_d [MeV]	m_u/m_d
value	1.9	4.6	0.42
statistics	0.0	0.0	0.00
lattice systematics	0.1	0.2	0.01
perturbative	0.1	0.2	–
EM	0.1	0.1	0.04

Table 1: Value of m_u/m_d calculated by the MILC Collaboration [1] and estimates of the different sources of error (with m_u and m_d determined in the $\overline{MS}$ scheme at 2 GeV). The row labeled “EM” shows the size of the error coming from a phenomenological estimate of electromagnetic contributions to the quark masses.

¹We do not include quark-mass renormalization effects due to the presence of the EM field, since they are much smaller than our precision.

$\approx a[\text{fm}]$	Volume	β	m_l/m_s	# configs.
0.12	$20^3 \times 64$	6.76	0.01/0.05	2254
	$28^3 \times 64$	6.76	0.01/0.05	274
	$20^3 \times 64$	6.76	0.007/0.05	1261
	$24^3 \times 64$	6.76	0.005/0.05	2099
0.09	$28^3 \times 96$	7.09	0.0062/0.031	1930
	$40^3 \times 96$	7.08	0.0031/0.031	1015
0.06	$48^3 \times 144$	7.47	0.0036/0.018	670

Table 2: Parameters of the asqtad ensembles used in this study.

we use the above expression plus the NNLO analytic terms. For investigating the finite volume effects, we include standard terms dependent on $m_\pi L_s$ from EM tadpoles, as well as an empirical EM finite volume correction in the form $f_v q_{xy}^2/L_s^2$ used previously in Ref. [7], where f_v is a constant and L_s is the spatial lattice size. However, as discussed below, our measured finite volume effects are rather small at present, and including or omitting the finite volume terms from the fits currently makes little difference in the final results.

2. Lattice setup

Our EM field on the lattice is “photon-quenched,” *i.e.*, the sea quarks are taken to be electromagnetically neutral, and the $U(1)_{\text{EM}}$ links are generated independently of the $SU(3)_{\text{QCD}}$ links. The fact that the photons are not present in the sea does not affect the NLO fits to the EM meson splittings since, as shown in Ref. [8], the unknown LEC controlling sea-quark mass dependence cancels in EM splittings between mesons with the same valence masses. There are physical NLO effects missing due to the absence of sea-quark charges, but these may be inserted after the fact since they appear only in chiral logarithm terms with known (LO) coefficients. Uncontrolled EM quenching effects do come in at NNLO, but should be negligible at the current level of precision. Because diagrams that have intermediate gluon or photon states (“quark-disconnected” diagrams) are difficult to compute on the lattice, and because of the photon quenching, we have to redefine the neutral pion on the lattice ${}'\pi^{0'}$ to have the mass:

$$m_{i\pi^{0'}}^2 = (m_{uu}^2 + m_{d\bar{d}}^2)/2, \quad (2.1)$$

where $u\bar{u}$ and $d\bar{d}$ are states with charges $(2/3e, -2/3e)$ and $(1/3e, -1/3e)$ and disconnected diagrams are dropped by fiat. The effect of the disconnected diagrams is expected to be small, since EM contributions to the neutral pion must in any case vanish in the chiral limit.

We calculate the meson spectrum on the set of asqtad ensembles with 2+1 flavors listed in Table 2 [1]. The values of the electron charge that we use are $e = \pm 0.909, \pm 0.606$ and $\pm 0.303, 0$, corresponding to $9\alpha_{\text{phys}}, 4\alpha_{\text{phys}}, \alpha_{\text{phys}}$ and 0.

3. Results

We do not see large finite volume effects in the EM splittings calculated on the $a \approx 0.12$ fm

ensembles with $L_s = 20$ and 28 . The volume effects do increase with the quark charges, but remain small. In Fig. 1 we compare our results with the finite volume effects for a charged kaon (with 3 times the physical charges) expected from the BMW collaboration result [7] (magenta error bar). We find that ours are about three times smaller. A similar comparison is shown in Fig. 3 for physically charged kaons. Nevertheless, the error on the finite volume effect in our data (computed simply by propagating the errors in the difference between the results on the two volumes) is slightly larger than the effect itself, so any tension with the BMW result is less than a 2σ effect. Indeed, we see no reason for any difference with BMW other than statistics, since as far as we can tell, we are treating the $U(1)_{\text{EM}}$ fields in the same way they do, and we do not expect the EM finite volume effects to be strongly dependent on quark mass or quark action. The finite volume effects we see are also smaller than those expected from the RBC Collaboration results [9], but in that case some or all of the difference may be due to the different treatment of zero modes in our $U(1)_{\text{EM}}$ fields. We are currently increasing the statistics on the $a \approx 0.12$ fm, $L_s = 28$ ensemble in hopes of clarifying this issue.

The taste splitting between the Goldstone pion and the second local pion grows with the quark charge for the neutral pions (see Fig. 2 for the two coarse ensembles with the same parameters and

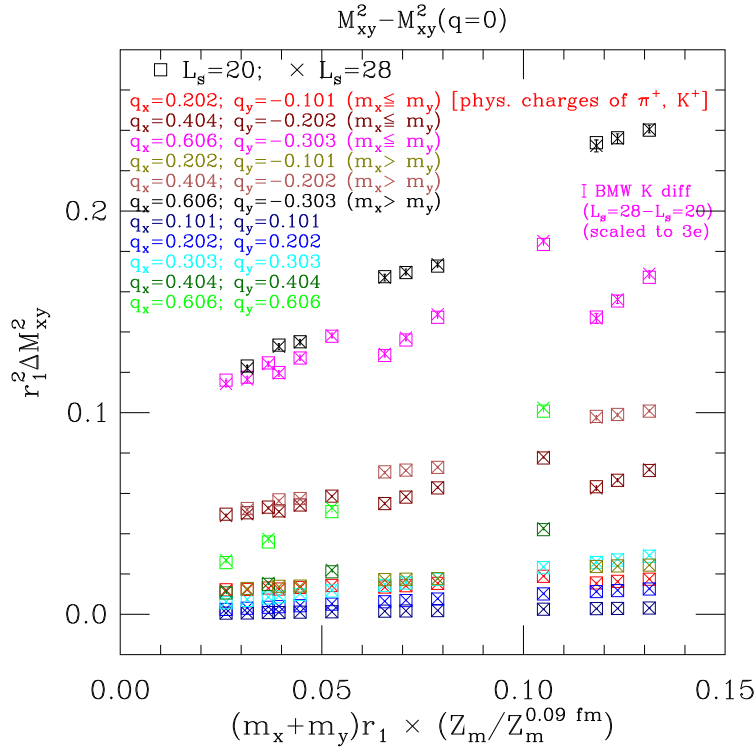


Figure 1: EM pseudoscalar splittings calculated on two coarse ensembles with $m_l/m_s = 0.01/0.05$ and spatial sizes $L_s = 20$ and $L_s = 28$ vs. the sum of the valence quark masses. The results for the different quark charge combinations are distinguished by color. The size of the finite volume effects found by the BMW group [7] is shown in magenta in the upper right and is scaled to charge $3e$, to correspond to our magenta points plotted slightly below that. The finite volume effects we see (difference between crosses and squares) are smaller than those found by BMW.

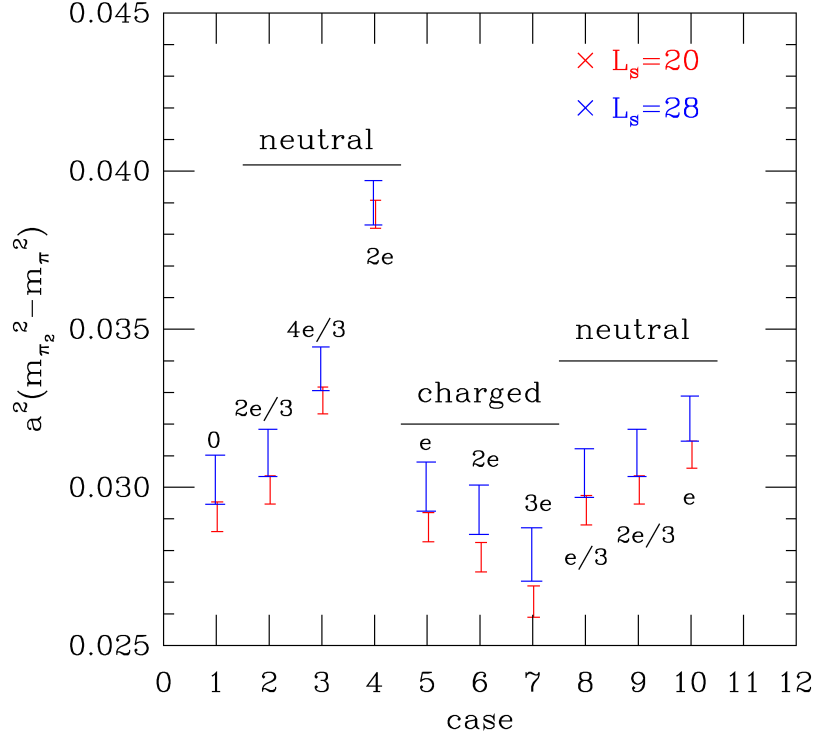


Figure 2: Taste splitting between the Goldstone pion and the second local pion on the coarse ensembles with $m_l/m_s = 0.01/0.05$ and $L_s = 20$ and $L_s = 28$. The x-axis values are arbitrary labels for the mesons with various values of the quark charges. Case 1 is a pion made from uncharged quarks. The first group of neutral pions (cases 2–4) are essentially $\bar{u}u$ combinations, and the second neutral group (cases 8–10) are of the $\bar{d}d$ type (the $(2e/3, -2e/3)$ combination appears in both neutral groups). These groups are labeled by one of the quark charges (the other has an opposite sign). The middle group (cases 5–7), has quark charges with the physical ratio of (2:1); they are labeled by the total meson charge.

different L_s in Table 2). This shows that, for charges larger than the physical charges, quark taste changing by high-momentum photons becomes a significant correction to that by high-momentum gluons. For charged pions, where annihilation into photons is forbidden, the effect is smaller (and negative), but still evident. The fit function Eq. (1.2) is based on the neglect of taste-violations caused by photons. For that reason, the analysis presented here focuses only on fits with physical quark charges. However, to the extent that photon-induced taste violations remain small compared with gluon-induced violations, which is arguably the case for all values of quark charges shown in Fig. 2, one should be able to expand the fit function in powers of α_{EM} . This would allow such effects to be included by adding α_{EM}^2 analytic terms to the fit function. We have made some preliminary fits along these lines to our full data set with quark charges up to three times the physical values, and they seem to work reasonably well.

Before leaving the subject of taste violations, we note that Fig. 2 shows that taste splitting is not very much affected by finite volume effects (compare the data in blue and red at $L_s = 20$ and 28 for the above coarse ensembles).

We now fit, to Eq. (1.2) plus NNLO analytic terms, the EM splitting of the meson spectrum

using the data with the physical electron charge e (i.e., mesons made from combinations of u and/or d quarks, with $q_u = 2/3e$ and $q_d = -1/3e$). Partially quenched points are included; in typical fits there are between 50 to 120 data points, with 20 to 30 fit parameters (depending on how many of the NNLO terms are included, and whether small variations with a^2 of the LO and NLO low energy constants are allowed). A typical fit is shown in Fig. 3, along with the unitary pions and kaons on each ensemble. The fit is uncorrelated: the covariance matrix is nearly singular, and the statistics are insufficient to determine it with enough precision to yield good correlated fits. Based on the fits, our preliminary determination of the correction to Dashen's theorem in the continuum limit and at physical quark mass is $\varepsilon = 0.65(7)(14)$, where the errors are statistical and systematic, respectively. The systematic error comes largely from variations in ε when the assumptions going into the chiral/continuum fit are changed. Systematic effects are still under investigation. In particular, based on the currently small finite volume effects seen in our data, we do not include a finite volume error here. However, we suspect that better statistics on our larger lattices will yield a statistically significant finite volume error. Our result is compatible with previous ones: $0.60(14)$ (statistics only) [10], $0.628(59)$ (statistics only) [9], and $0.70(4)(8)$ [7]. With our value for ε from above, our preliminary estimate for the EM uncertainty in m_u/m_d is reduced to 0.022 [11], which is about half of our previous error shown in Table 1.

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References

- [1] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010), [arXiv:0903.3598 [hep-lat]]; C. Aubin *et al.* [MILC Collaboration], Phys. Rev. D **70**, 114501 (2004), [arXiv:hep-lat/0407028]; A. Bazavov *et al.* [The MILC Collaboration], PoS(LAT2009)079 (2009), [arXiv:0910.3618].
- [2] S. Basak *et al.* [MILC Collaboration], PoS(LAT2008)127 (2008), [arXiv:0812.4486 [hep-lat]].
- [3] C. Bernard and E. D. Freeland, PoS LATTICE **2010**, 084 (2010), [arXiv:1011.3994 [hep-lat]].
- [4] A. Torok *et al.*, PoS LATTICE **2010**, 127 (2010).
- [5] R. Dashen, Phys. Rev. **183**, 1245 (1969).
- [6] G. Colangelo *et al.*, Eur. Phys. J. C **71**, 1695 (2011) [arXiv:1011.4408 [hep-lat]].
- [7] A. Portelli *et al.*, [arXiv:1201.2787 [hep-lat]].
- [8] J. Bijnens and N. Danielsson, Phys. Rev. D **75**, 014505 (2007) [hep-lat/0610127].
- [9] T. Blum *et al.*, Phys. Rev. D **82**, 094508 (2010) [arXiv:1006.1311 [hep-lat]].

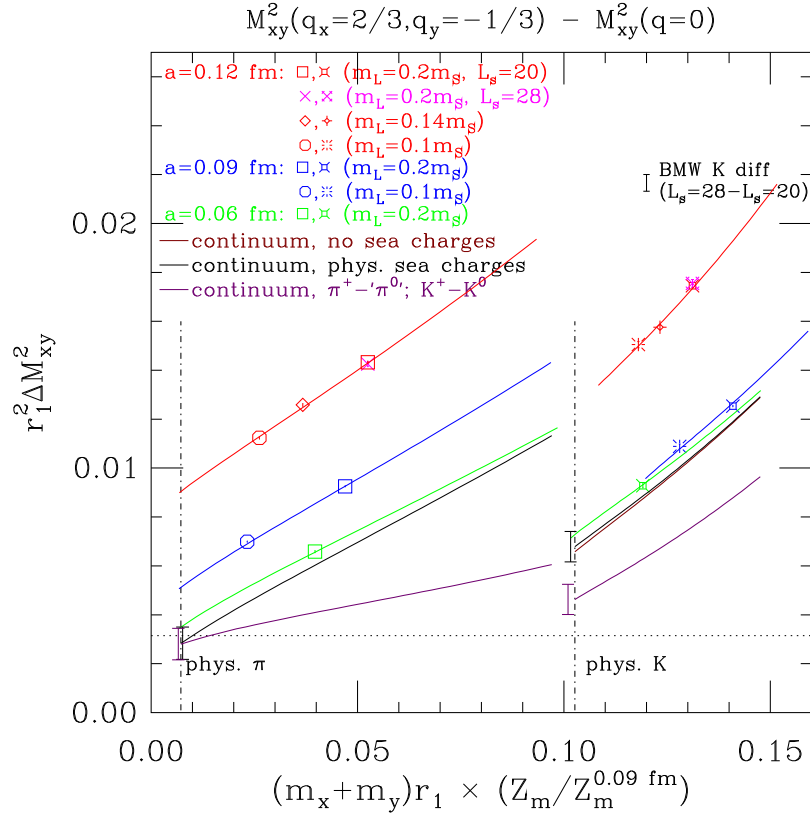


Figure 3: Our preliminary results for electromagnetic corrections in pseudoscalar mesons. Plotted is the difference in the squared mass of mesons with charged valence quarks and neutral valence quarks vs. the sum of the valence quark masses. Only a small subset of the data that was used in the fit is shown in the plot. This fit had 55 data points, 26 parameters, and an (uncorrelated) p value of 0.09. The red, blue and green curves correspond to three different lattice spacings and include the effects of taste breaking. The vertical dot-dashed lines correspond to the quark masses of the π and K mesons. The purple curves are the continuum limits for $K^+ - K^0$, and for $\pi^+ - \pi^{0'}$ (left), where the $\pi^{0'}$ is the average of a neutral pion with charges $(2/3e, -2/3e)$ and $(1/3e, -1/3e)$. The latter is an approximation to the physical π^0 , which would also be affected by quark annihilation terms not included in our calculation. The horizontal dotted line is the physical value of the pion electromagnetic mass splitting and is in close agreement with our calculation. The result for the K is larger than for the pion, giving a correction to the lowest order of Dashen's theorem by a factor of $\varepsilon = 0.65(7)$. In the upper right we show the expected size of finite volume effects for the kaon from the BMW calculation [7]. It should be compared with the (tiny) difference between the red square and magenta cross, or 'fancy' red square and 'fancy' magenta cross.

- [10] A. Portelli *et al.* [Budapest-Marseille-Wuppertal Collaboration], PoS LATTICE **2010**, 121 (2010) [arXiv:1011.4189 [hep-lat]].
- [11] D. Toussaint, PoS(Lattice 2012)159.
- [12] M. A. Clark *et al.*, Comput. Phys. Commun. 181, 1517 (2010) [arXiv:0911.3191 [hep-lat]]. R. Babich *et al.*, International Conference for High Performance Computing, Networking, Storage and Analysis (SC), 2011 [arXiv:1109.2935 [hep-lat]].

Pseudoscalar meson physics with four dynamical quarks

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We present preliminary results for light, strange and charmed pseudoscalar meson physics from simulations using four flavors of dynamical quarks with the highly improved staggered quark (HISQ) action. These simulations include lattice spacings ranging from 0.15 to 0.06 fm, and sea-quark masses both above and at their physical value. The major results are charm meson decay constants f_D , f_{D_s} and f_{D_s}/f_D and ratios of quark masses. This talk will focus on our procedures for finding the decay constants on each ensemble, the continuum extrapolation, and estimates of systematic error.

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^{*}Speaker.

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1. Introduction

Lattice calculations of pseudoscalar meson decay constants, when combined with measured nonleptonic decay rates, can be used to extract CKM matrix elements and test the Standard Model. The lattice calculation includes a determination of the quark masses — fundamental parameters of the Standard Model. Here we present preliminary results for the charm meson decay constants f_D and f_{D_s} , and the ratios of quark masses m_c/m_s and m_u/m_d .

These calculations use lattices generated with the one-loop and tadpole improved Symanzik gauge action [1] and the HISQ fermion action [2]. We include four flavors of dynamical sea quarks: degenerate up and down, strange, and charm. Iterated smearing in the HISQ action reduces taste violations by a factor of three relative to the asqtad action. An improved charm-quark dispersion relation allows us to treat it the same way as the lighter quarks. Our lattice ensembles include ensembles with approximately physical light-quark masses, with volumes as large as 5.6^3 fm^3 . For more details, see Refs [3, 4, 5]. The parameters of the ensembles used in this calculation are tabulated in J. Kim’s talk [6]. In the first stage of analysis we fit pseudoscalar meson two-point correlators to extract masses and amplitudes from random wall operators for a set of valence-quark masses. (See Ref. [6].) In the second stage of the analysis, we interpolate or extrapolate in valence-quark masses to find the tuned valence masses on each ensemble, and the decay constants evaluated at these valence masses, but at the sea-quark masses and lattice spacing of the individual ensemble. Then we combine the results of the different ensembles to make a continuum extrapolation and corrections for mistuned sea-quark masses.

We use the pion decay constant f_π to set the scale. Since this is determined from the same set of correlators as the charm meson decay constants, the analysis is self-contained in the sense that we do not need an intermediate quantity such as r_0 or r_1 found in a separate analysis. This reduces the error from determining the lattice spacing, and simplifies the error analysis. Ensembles with physical light-quark masses dominate the analysis and allow a simple interpolation to adjust for light-quark mass corrections. However, it is likely that use of staggered chiral perturbation theory will lead to better controlled fits, and J. Komijani’s talk describes progress in this direction [7].

2. Decay constants on each ensemble

In the first stage of the analysis [6] we determine the masses and amplitudes for the two-point pseudoscalar correlators for a set of valence quark masses on each ensemble. These masses include 0.9 and 1.0 times the sea charm quark mass, 0.8 and 1.0 times the sea strange-quark mass, and a range of lighter masses. Since the sea-quark masses were estimated before the production runs began, they are inevitably slightly mistuned. In the second stage of the analysis we determine tuned quark masses for each ensemble, and evaluate the decay constants at these valence-quark masses. Our primary analysis uses f_π to fix the lattice spacing, and proceeds as follows. To estimate statistical errors, this whole procedure is done inside a jackknife resampling.

1. Interpolate or extrapolate in the light valence-quark mass m_l to the point where M_π/f_π has its physical¹ value. This fixes am_l and the lattice spacing a .
2. Interpolate or extrapolate in valence strange-quark mass am_s to where $2M_K^2 - M_\pi^2$ has its physical value. This fixes m_s .

¹adjusted for E&M and finite size — see later

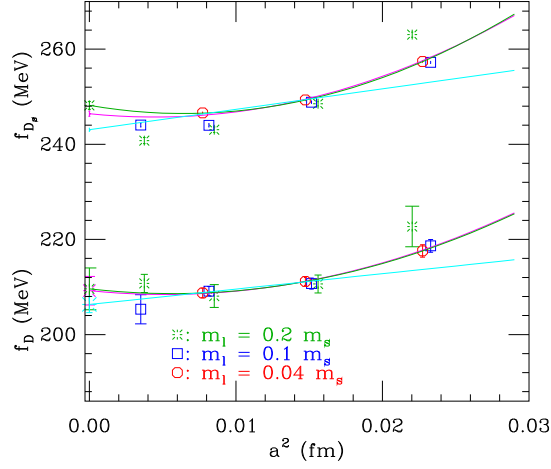


Figure 1: f_D and f_{D_s} on the different ensembles. Fits that are quadratic and linear in a^2 , or use only physical quark mass ensembles are superimposed on the data. More details are given in the text.

3. Interpolate or extrapolate to the charm valence mass where M_{D_s} is correct. This fixes m_c .
4. Find $m_d - m_u$ from E&M adjusted $K^0 - K^+$ mass difference [8]
5. Find, by interpolation or extrapolation, f_K at the adjusted up-quark mass.
6. Find f_D and M_D (a check) at the adjusted down and charm masses.
7. Find f_{D_s} at the adjusted strange and charm masses.
8. Find M_{η_c} (check) at the adjusted charm-quark mass.

We have also used a tuning procedure where we replaced f_π and M_π by the decay constant, $f_{p_{4s}}$, and mass, $M_{p_{4s}}$, of a fictitious meson with degenerate valence quark masses at 0.4 times the strange-quark mass, using the values for $f_{p_{4s}}$ and $M_{p_{4s}}$ in MeV determined from three flavor asqtad data. Finally, we varied the procedure by first fixing the lattice spacing from the static-quark potential, and then tuning the valence quark masses as described above.

In Eq. 2.1 we list results from the above procedure for the most influential ensemble ($a \approx 0.09$ fm with physical masses). These results are adjusted for finite size and some electromagnetic effects, but are not adjusted for mistuned sea-quark masses or extrapolated to the continuum limit. The errors here are statistical only but, as discussed above, errors from scale setting and valence-quark mass tuning are included in the statistical error here. The D^+ , D^0 and η_c masses are not used in the tuning, so they can be compared to their experimental values, shown in parentheses.

$$\begin{aligned}
 a &= 0.08792(10) \text{ fm} & am_l &= 0.001333(5) & am_s &= 0.03648(11) & am_c &= 0.4323(7) \\
 m_u/m_d &= 0.480(6) & m_s/m_l &= 27.36(3) & m_c/m_s &= 11.851(17) \\
 f_K &= 155.12(22) \text{ MeV} \\
 M_{D_0} &= 1867.8(1.5) \text{ MeV (cf 1864.8)} & M_{D^+} &= 1870.2(1.2) \text{ MeV (cf 1869.6)} \\
 M_{\eta_c} &= 2980.2(3) \text{ MeV (cf 2980.3(1.2))} \\
 f_D &= 208.75(1.03) \text{ MeV} & f_{D_s} &= 246.60(20) \text{ MeV} & f_{D_s}/f_D &= 1.181(6)
 \end{aligned} \tag{2.1}$$

3. Continuum extrapolation

The results for f_D and f_{D_s} on each ensemble are shown in Fig. 1. In this figure the physical quark mass ensembles, labelled as “ $m_l = 0.04m_s$ ”, have the smallest statistical errors. This is

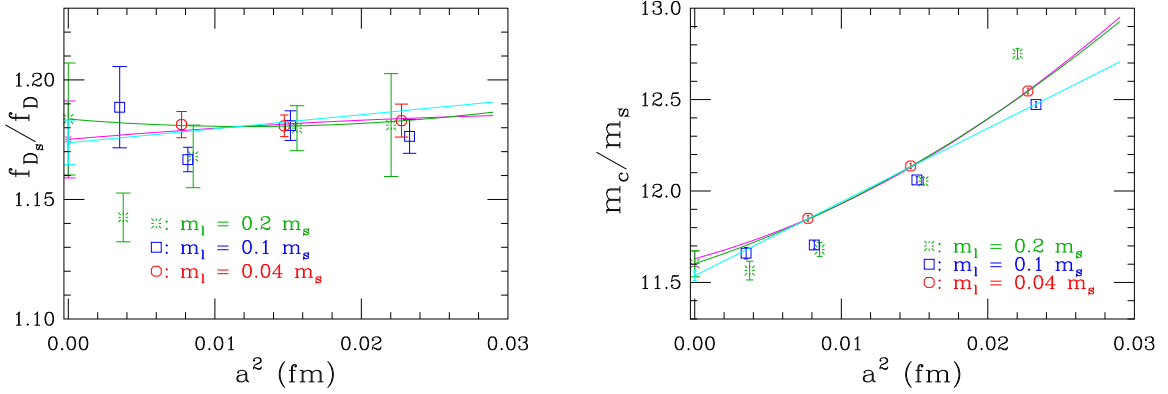


Figure 2: The ratios f_{D_s}/f_D (left panel) and m_c/m_s (right panel) on the different ensembles. The superimposed fit functions are the same forms as in Fig. 1.

due to their larger physical volumes, where the random wall and Coulomb wall sources, together with the average over spatial position of the sink operator, result in better statistics. Errors are large on some of the $m_l = 0.2 m_s$ ensembles because the lightest valence-quark mass used on these ensembles was $0.1 m_s$, so a significant extrapolation in valence light-quark mass was necessary. When these points are fit to functions of lattice spacing and sea-quark mass, the physical quark mass points dominate the fit. Indeed, we could get reasonable results by simply using the physical quark mass ensembles. In practice, we use the physical quark mass and the $m_l = 0.1 m_s$ ensembles, where the $m_l = 0.1 m_s$ ensembles allow correction for mistuning of the light sea-quark masses in the physical quark mass ensembles and, because of the $m_l = 0.1 m_s$ ensemble at lattice spacing $a \approx 0.06$ fm, help to determine the dependence on the lattice spacing.

Figure 1 shows three different fits to this data. The magenta line uses all four of the lattice spacings, and is quadratic in a^2 and linear in light sea-quark mass. The straight cyan line in Fig. 1 omits the $a = 0.15$ fm points, and is linear in both a^2 and $m_{l,\text{sea}}$. The green line is a quadratic fit using only the physical quark mass points, with small adjustments to correct for sea-quark mass mistuning. The symbols at $a = 0$ are the continuum limits of these fits, showing the statistical error. The size of these symbols is proportional to the p -value of the fit, with the symbol size in the graph legend corresponding to 50%. Since we expect both order a^2 and a^4 corrections to the data, and since some other accurately determined quantities such as the mass of the η_c clearly need a^4 terms to fit the results, we take the quadratic fit results as our central value, with the larger of the difference between the quadratic and linear fits or the difference between the quadratic and physical-quark-mass-only fits as an estimate of the systematic error coming from our choice of fit form.

Figure 2 shows, with the same notation, the ratios f_{D_s}/f_D and m_c/m_s on each ensemble, together with fits to the same functional forms and ranges of data as in Fig. 1.

4. Systematic errors

Statistical errors from the jackknife analysis incorporate errors in lattice spacing determination and valence-quark mass tuning, since this tuning is redone for each jackknife sample. The following additional systematic errors are included in our error budget.

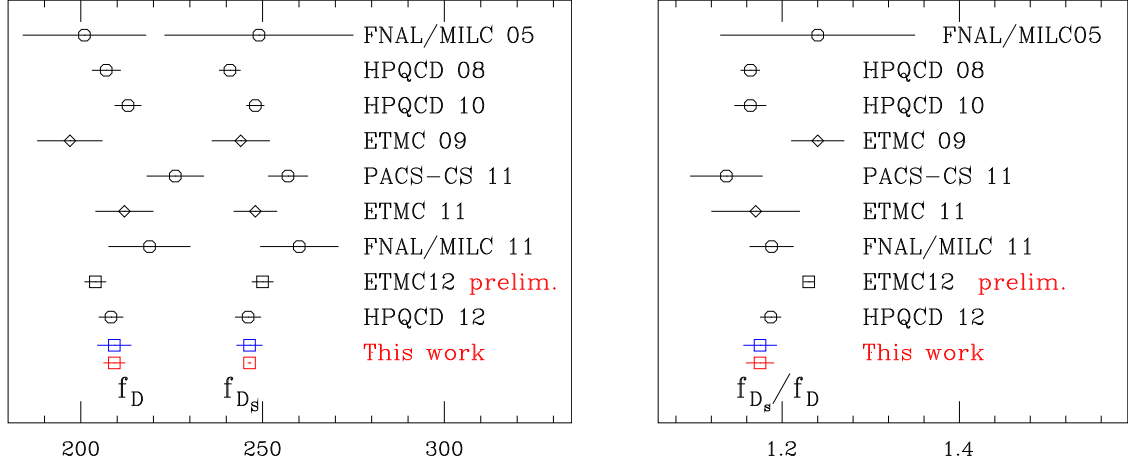


Figure 3: Comparison of lattice results for f_D and f_{D_s} (left panel) and for f_{D_s}/f_D (right panel). Results are from Ref. [10] and this work. Diamonds represent results with 2, octagons with 2+1, and squares with 2+1+1 dynamical flavors. For this work the red error bars (lower) are statistical only, while the blue error bars (higher) include systematic error estimates.

Effects of excited states in the two-point correlators were estimated by varying the time range in the fits and the priors for excited state masses with reasonable ranges [6].

Effects of finite spatial size were tested by running otherwise identical ensembles with three different spatial sizes. This was done at $a \approx 0.12$ fm with $m_l/m_s = 1/10$. The results, summarized in Fig. 4, show that the significant effects are in the light pseudoscalar sector, on M_π , f_π and f_K , and that chiral perturbation theory is a reasonable guide. From these results, we estimated the effects on M_π , f_π and f_K at the physical light-quark mass in a 5.5 fm box. (Since our fits are evaluated at this mass, it doesn't matter that the ensembles with other sea-quark masses would have different finite-size effects.) Then, in the analysis procedure described in section 2, we used the values of M_π , f_π and f_K adjusted to this size box. (That is, we compute $f_K/f_\pi(5.5 \text{ fm})$ etc.) Afterwards, we use these same factors to correct the computed f_K back to its infinite volume value. We use the values with the finite-size adjustments as our central values, and take one half of the shifts when these adjustments are omitted as a remaining systematic error.

The effects of electromagnetic interactions and isospin breaking ($m_u \neq m_d$) are considered together. We tune using the π^0 mass, where electromagnetic and isospin breaking effects are expected to be small. Then we use a separate calculation of electromagnetic effects on the kaon mass [8], whose main result is parameterized in terms of a violation of Dashen's theorem

$$M_{K^+,\text{adj}}^2 = M_{K^+}^2 - (1 + \Delta_{\text{EM}}) (M_{\pi^+}^2 - M_{\pi^0}^2) \quad . \quad (4.1)$$

Here $M_{K^+,\text{adj}}$ is the K^+ mass adjusted to remove the effects of electromagnetism, and the result of Ref. [8] is $\Delta_{\text{EM}} = 0.65(26)$. Then, in tuning the strange-quark mass from $2M_K^2 - M_\pi^2$, we use the average squared kaon mass $M_K^2 = (M_{K^+,\text{adj}}^2 + M_{K^0}^2)/2$. We also use this result combined with our meson mass measurements to determine the up-down quark mass difference,

$$a^2 (M_{K^0}^2 - M_{K^+,\text{adj}}^2) = a(m_d - m_u) \frac{\partial (aM_K)^2}{\partial am_l} \quad , \quad (4.2)$$

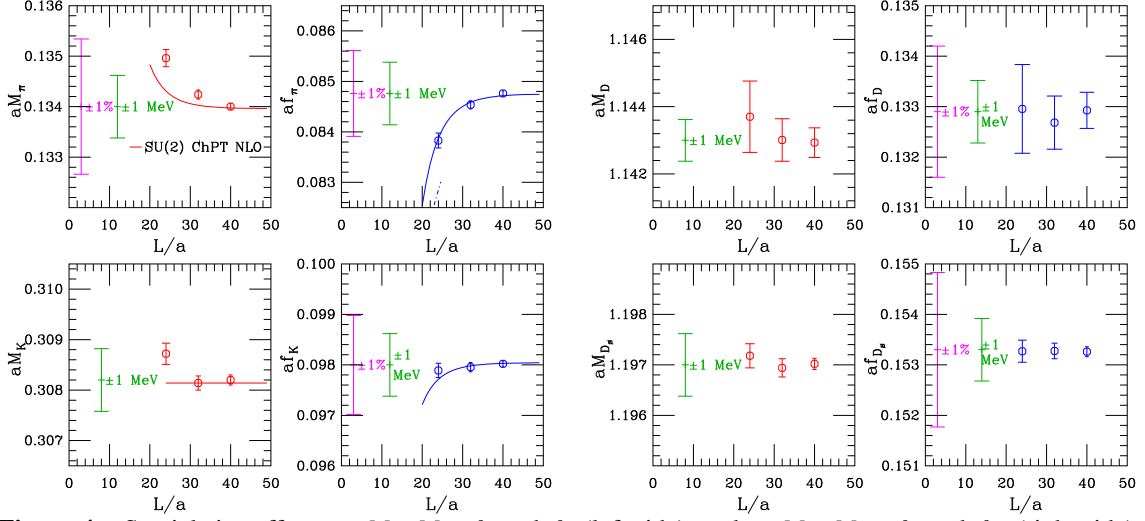


Figure 4: Spatial size effects on M_π , M_K , f_π and f_K (left side), and on M_D , M_{D_s} , f_D and f_{D_s} (right side). Solid lines are the one loop chiral perturbation theory forms. To show the magnitude of the effects, green error bars show an arbitrary value ± 1 MeV, and magenta error bars $\pm 1\%$.

Source	f_D	f_{D_s}	f_{D_s}/f_D	m_c/m_s	m_u/m_d
Statistics	3.0 MeV	0.5 MeV	0.016	0.041	0.009
Excited	0.5 MeV	0.5 MeV	0.004	0.005	0.003
Volume	0.3 MeV	0.2 MeV	0.0004	0.008	0.0005
E&M	0.04 MeV	0.12 MeV	0.001	0.001	0.021
Scale setting	2.0 MeV	1.3 MeV	0.003	0.02	0.023
a^2 fit form	2.9 MeV	3.3 MeV	0.010	0.09	0.011

Table 1: Error budget: The statistical error includes error from valence-quark mass tuning and from a continuum extrapolation with fixed fit form. Estimation of the systematic error is discussed in the text.

where $\frac{\partial M_K^2}{\partial m_l}$ is obtained from the difference in M^2 between the two lightest valence-quark masses, with the strange mass set at the sea strange mass. We estimate the remaining systematic errors from electromagnetism by combining, in quadrature, the effects of changing Δ_{EM} by one standard deviation with the effects of shifting the average kaon mass squared by 900 MeV², which is the full result of a preliminary computation of electromagnetic effects on this quantity [8]. When computing f_D , the light valence-quark mass is interpolated to the resulting down-quark mass, and similarly for other quantities involving valence up and down quarks. We expect that the effects of electromagnetic interactions and isospin violation in the sea quarks are small, and ignore them.

Errors from the scale setting and quark mass tuning procedure are estimated from the change in results when r_1 or f_{p4s} are used to set the scale instead of f_π .

5. Conclusions

We find preliminary results $f_D = 209.2(3.0)(3.6)$ MeV, $f_{D_s} = 246.4(0.5)(3.6)$ MeV, $f_{D_s}/f_D = 1.175(16)(11)$, $m_c/m_s = 11.63(4)(9)$ and $m_u/m_d = 0.505(9)(33)$. Our results are consistent with those of other collaborations [10], and the errors are comparable to the most precise published calculation by HPQCD. In the future we will further reduce the error by using staggered chiral

perturbation theory, which will allow us to make better use of the correlators with unphysical valence-quark masses [7], and by the addition of an ensemble with physical sea-quark masses at a lattice spacing of 0.06 fm.

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References

- [1] K. Symanzik, In: *Recent Developments in Gauge Theories*, edited by G. 't Hooft et al. (Plenum Press, New York, 1980), p. 313, (1980); K. Symanzik, *Nucl. Phys.* **B226**, 187 (1983); M. Lüscher and P. Weisz, *Phys. Lett.* **B158**, 250 (1985); M. Lüscher and P. Weisz, *Commun. Math. Phys.* **97**, 59 (1985); M.G. Alford *et al.*, *Phys. Lett.* **B361**, 87 (1995).
- [2] E. Follana *et al.*, *Nucl. Phys. B (Proc. Suppl.)* **129** and **130**, 447 (2004) [arXiv:hep-lat/0311004]; E. Follana *et al.*, *Nucl. Phys. B. (Proc. Suppl.)* **129** and **130**, 384, 2004 [arXiv:hep-lat/0406021]; E. Follana *et al.*, (HPQCD/UKQCD Collaboration) *Phys. Rev.* **D75**, 054502 (2007) [arXiv:hep-lat/0610092].
- [3] A. Bazavov *et al.* (MILC Collaboration), *Phys. Rev. D* **82**, 074501 (2010), [arXiv:1004.0342].
- [4] A. Bazavov *et al.* (MILC Collaboration), *PoS (Lattice 2010) 320* (2010), [arXiv:1012.1265].
- [5] A. Bazavov *et al.* (MILC Collaboration) in preparation.
- [6] A. Bazavov *et al.* (MILC Collaboration), *PoS (Lattice2012) 158*.
- [7] J. Komijani and C. Bernard (MILC Collaboration), *PoS (Lattice2012) 199*.
- [8] L. Levkova *et al.* (MILC Collaboration), *PoS (Lattice2012) 137*; C. Bernard *et al.*, *PoS (CD12) 030*, *Proceedings of Chiral Dynamics 2012*, in preparation.
- [9] C. Aubin *et al.* (Fermilab lattice and MILC Collaborations), *Phys. Rev. Lett.* **95**, 122002(2005), [arXiv:hep-lat/0506030].
- [10] E. Follana *et al.* (HPQCD Collaboration), *Phys. Rev. Lett.* **100**, 062002 (2008), [arXiv:0706.1726]; C. Davies *et al.* (HPQCD Collaboration), *Phys. Rev. D* **82**, 114504 (2010), [arxiv:1008.4018]; B. Blossier *et al.* (ETMC Collaboration), *JHEP* **0907** 043 (2009), [arXiv:0904.0954]; Y. Namekawa *et al.* (PACS-CS Collaboration), *Phys. Rev. D* **84** (2011) 074505, [arXiv:1104.4600]; P. Dimopoulos *et al.* (ETMC Collaboration), *JHEP* **01**, 046 (2012), [arXiv:1107.1441]; J.A. Bailey *et al.* (Fermilab Lattice and MILC Collaborations), *PoS (Lattice2011) 320* [arXiv:1112.3978]; A. Bazavov *et al.* (Fermilab Lattice and MILC Collaborations), *Phys. Rev. D* **85** 114506 (2012) [arXiv:1112.3051]; K. Jansen, BNL workshop “New Horizons for Lattice Computations with Chiral Fermions,” <http://www.bnl.gov/ltc2012/> (2012); H. Na *et al.* (HPQCD Collaboration), *PoS (Lattice2012) 102*; H. Na *et al.* (HPQCD Collaboration), *Phys. Rev. D* **85** 125029 (2012) [arXiv:1206.4936].

Kaon semileptonic decay form factors with HISQ valence quarks

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Fermilab Lattice and MILC Collaborations

We report on the status of our kaon semileptonic form factor calculations using the highly-improved staggered quark (HISQ) formulation to simulate the valence fermions. We present results for the form factor $f_+^{K\pi}(0)$ on the asqtad $N_f = 2 + 1$ MILC configurations, discuss the chiral-continuum extrapolation, and give a preliminary estimate of the total error. We also present a more preliminary set of results for the same form factor but with the sea quarks also simulated with the HISQ action; these results include data at the physical light quark masses. The improvements that we expect to achieve with the use of the HISQ configurations and simulations at the physical quark masses are briefly discussed.

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1. Introduction and methodology

The study of exclusive semileptonic decays of D and K mesons provides a way of extracting the Cabibbo-Kobayashi-Maskawa (CKM) matrix elements $|V_{cd(cs)}|$ and $|V_{us}|$ with errors competitive with those obtained using other methods such as leptonic decays, neutrino-antineutrino interactions, or τ decays. Comparison of the values obtained with different methods could reveal new physics (NP) effects, and comparison of the shape of the form factors describing those exclusive decays with experiment can provide a check of the lattice methodology employed.

Our program includes analyzing $K \rightarrow \pi l \nu$ and $D \rightarrow K(\pi) l \nu$ semileptonic decays at zero as well as non-zero momentum transfer. In these proceedings we focus on the status of the $K \rightarrow \pi l \nu$ analysis at zero momentum transfer, which one can combine with experimental data to extract the CKM matrix element $|V_{us}|$. The limiting error currently comes from the lattice determination of the form factors defined in (1.1) [1]. A precise determination of $|V_{us}|$ provides stringent tests of first-row unitarity and gives information about the scale of new physics [2].

The theory input needed to extract the CKM matrix elements from exclusive semileptonic widths are form factors parametrizing the corresponding hadronic matrix elements:

$$\langle P_2 | V^\mu | P_1 \rangle = f_+^{P_1 P_2}(q^2)(p_{P_1} + p_{P_2} - \Delta)^\mu + f_0^{P_1 P_2}(q^2)\Delta^\mu, \quad (1.1)$$

where $\Delta^\mu = (m_{P_1}^2 - m_{P_2}^2)q^\mu/q^2$, $q = p_{P_1} - p_{P_2}$, and V is the appropriate flavor-changing vector current. We obtain the needed form factor $f_+^{K\pi}(0)$ using the relation $f_0^{K\pi}(q^2) = \frac{m_s - m_l}{m_K^2 - m_\pi^2} \langle \pi | S | K \rangle(q^2)$, and the fact that $f_+(0) = f_0(0)$ due to the kinematic constraint. This method [3] allows us to eliminate the need for a renormalization factor and to extract the form factor from three-point correlation functions with insertion of a scalar current instead of a vector current.

The momentum transfer of the three-point functions is tuned to zero or very close to zero using twisted boundary conditions to inject external momentum [4]. The general structure of the correlation functions is given in Fig. 1. We consider either a moving π ($\theta_0 = \theta_1 = 0$ and $\theta_2 \neq 0$) or a moving K ($\theta_0 = \theta_2 = 0$ and $\theta_1 \neq 0$), for $K \rightarrow \pi l \nu$.

2. HISQ valence fermions and asqtad $N_f = 2 + 1$ configurations

For the first analysis we use the asqtad $N_f = 2 + 1$ MILC configurations and the HISQ action to simulate the valence quarks. The strange valence-quark mass is fixed to its physical value and the light valence-quark mass is fixed so $\frac{m_l^{\text{val}}(\text{HISQ})}{m_s^{\text{phys}}(\text{HISQ})} = \frac{m_l^{\text{sea}}(\text{asqtad})}{m_s^{\text{phys}}(\text{asqtad})}$. The parameters of the ensembles included in this calculation and the details of the simulations we perform are collected in Table 1.

In order to extract the value of the form factor $f_+^{K\pi}(0) = f_0^{K\pi}(0)$, we perform a simultaneous fit of the relevant three- and two-point functions. The correlator fits and the multiple checks performed on their stability under the change of parameters, time range, number of exponentials in the fitting functions, and correlators included, was described in last year's conference proceedings [5]. The

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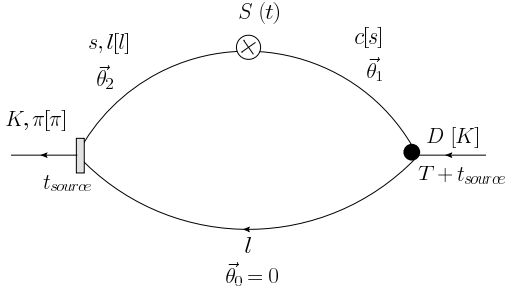


Figure 1: Structure of the 3-point functions needed to calculate $f_0^{DK(\pi)}[f_0^{K\pi}]$. Light quark propagators are generated at t_{source} with random wall sources. An extended charm [strange] propagator is generated at $T + t_{\text{source}}$.

$\approx a$ (fm)	am_l/am_h	N_{conf}	N_{sources}	N_T
0.12	0.020/0.050	2052	4	5
	0.010/0.050	2243	4	8
	0.07/0.050	2109	4	5
	0.05/0.050	2098	8	5
0.09	0.0124/0.031	1996	4	5
	0.0062/0.031	1946	4	5

Table 1: Aqstad nsembles and simulation details. am_h is the nominal strange-quark mass in the sea sector, N_{sources} is the number of time sources, and N_T the number of sink-source separations.

conclusion is that we find it very difficult to make changes in the fitting procedure that change the fit results outside the one sigma range. The only change with respect to last year's fits is that in our final correlator fits we are including functions with the momentum injected in both the π and in the K . The results from these combined fits for the different ensembles are shown in Fig. 2. Statistical errors are very small, $\sim 0.1 - 0.15\%$.

2.1 Chiral-continuum extrapolations

We need to extrapolate our results to the continuum limit and the physical light-quark masses, and also adjust for the mistuning of the strange sea-quark mass in the asqtad $N_f = 2 + 1$ MILC configurations. Our plan is to perform these extrapolations using partially quenched staggered chiral perturbation theory (S χ PT) at NLO plus regular continuum χ PT at NNLO. Addressing staggered effects at NLO should be enough to achieve the sub-percent precision that we target.

In the continuum, the form factor is given by $f_+^{K\pi}(0) = 1 + f_2 + f_4 + f_6 + \dots$, where, according to the Ademollo-Gatto (AG) theorem, the chiral corrections $f_2, f_4, f_6 \dots$ go to zero in the $SU(3)$ limit as $(m_K^2 - m_\pi^2)^2$. This means that at NLO there are no free low-energy constants and f_2 is fixed in terms of experimental quantities. At finite lattice spacing, however, we would have violations of the AG theorem due to discretization effects in the continuum dispersion relation needed to derive the relation between $f_0^{K\pi}(0)$ and the correlation functions we are generating.

The general structure of the fitting function we plan to use for our chiral fits is thus

$$f_+^{K\pi}(0) = 1 + f_2^{PQ,stag.}(a) + C_4^{(a)} \left(\frac{a}{r_1} \right)^2 + f_4^{cont.}(\text{logs}) + f_4^{cont.}(L_i) + r_1^4 (m_\pi^2 - m_K^2)^2 \left[C_6'^{(1)} + C_6^{(a)} \left(\frac{a}{r_1} \right)^2 \right], \quad (2.1)$$

where the constants $C_4^{(a)}$, $C_6^{(a)}$, and $C_6'^{(1)} \propto C_{12} + C_{34} - L_5^2$ are free parameters to be fixed by the chiral fits. The L_i 's are the usual $\mathcal{O}(p^4)$ low-energy constants (LEC's), and the C_{ij} are $\mathcal{O}(p^6)$ LEC's defined in [7]. The function $f_2^{PQ,stag.}(a)$ is the NLO partially quenched S χ PT expression, which incorporates the dominant lattice artifacts from taste breaking. To a very good approximation, there are no free parameters in that function. The taste-splitting and the taste-violating hairpin parameters

are already available for both the valence and the sea quarks from lattice calculations for asqtad or HISQ fermions, respectively. We are also in the process of calculating the taste-splittings for the mixed mesons, those made of one sea fermion and one valence fermion. The only parameter that we do not get from other calculations is an extra taste-violating hairpin parameter that appears due to the fact that we have a mixed action. We need to leave this quantity as a free parameter of the fit, although we expect its impact to be small. We take the NNLO contribution, f_4 , from the calculation in [6]. Finally, we try to include terms proportional to a^2 with free parameters $C_4^{(a)}$ (to take into account the violations of the AG theorem at finite lattice spacing) and $C_6^{(a)}$ (to account for the residual a^2 dependence at higher orders).

Since we have not completely checked the NLO partially quenched $S\chi$ PT calculation, here we use a simplified version without hairpin terms. We also approximate the taste-splittings of the mixed action mesons by the average of the sea and the valence values, $\Delta_{\text{mix}} = (\Delta_{\text{sea}}(\text{asqtad}) + \Delta_{\text{valence}}(\text{HISQ}))/2$ (we checked that using the preliminary values for the correct splitting does not change the extrapolated $f_+^{K\pi}$ by more than 0.1%). With these simplifications, we tried several variations of the fitting function in (2.1): fixing the LEC's L_i 's to their value from the global fit in [8], fixing them to the value from the fits in [9], or leaving the L_i 's as free parameters in the fit with prior central values equal to the results in [8] and varying the prior widths from the errors in [8] to an order of magnitude larger; including only the term proportional to $C_4^{(a)}$, the one proportional to $C_6^{(a)}$, or both, etc. The extrapolated value for $f_+^{K\pi}(0)$ has statistical errors between 0.2% and 0.3% in all cases and the different results agree with each other within one statistical σ . The violations of the AG theorem are around $0.32 - 0.15\%$ for $a \approx 0.12$ fm and $0.15 - 0.1\%$ for $a \approx 0.09$ fm. A typical example of the fits we have performed is shown in the left side of Fig. 2.

In order to check the impact of the choice of fitting function in the extrapolation, we have also done a number of fits replacing the NNLO continuum χ PT functions by a NNLO analytical parametrization

$$f_+^{K\pi}(0) = 1 + f_2^{PQ, \text{stag.}} + C_4^{(a)} \left(\frac{a}{r_1} \right)^2 + r_1^4 (m_\pi^2 - m_K^2)^2 \left[C_6^{(1)} (r_1 m_\pi)^2 + C_6^{(2)} (r_1 m_K)^2 \right. \\ \left. + C_6^{(3)} (r_1 m_\pi)^2 \ln(m_\pi^2/\mu^2) + C_6^{(4)} (r_1 m_\pi)^4 + C_6^{(a)} \left(\frac{a}{r_1} \right)^2 \right], \quad (2.2)$$

where $f_2^{PQ, \text{stag.}}$ is the same partially quenched NLO $S\chi$ PT expression as in (2.1) and the $C_4^{(a)}$, $C_6^{(a)}$, and $C_6^{(i)}$ with $i = 1 - 4$ are the free parameters in the fit. Again, we tried variations of the functional form in (2.2), turning on and off different NNLO and a^2 terms, and parametrizing them in different ways. All the fitting functions we tried in this category gave results within one statistical σ of each other. In the right-hand side of Fig. 2 we plot an example of these fits. Both methods to describe NNLO contributions give results that, again, agree within one statistical σ .

3. Preliminary results with HISQ valence quarks and HISQ $N_f = 2 + 1 + 1$ configurations

The second stage of our semileptonic decay program is the study of decays with $q^2 = 0$ for D and K mesons using HISQ for the valence and the sea quarks, *i.e.*, simulating on the HISQ $N_f = 2 + 1 + 1$ MILC configurations.

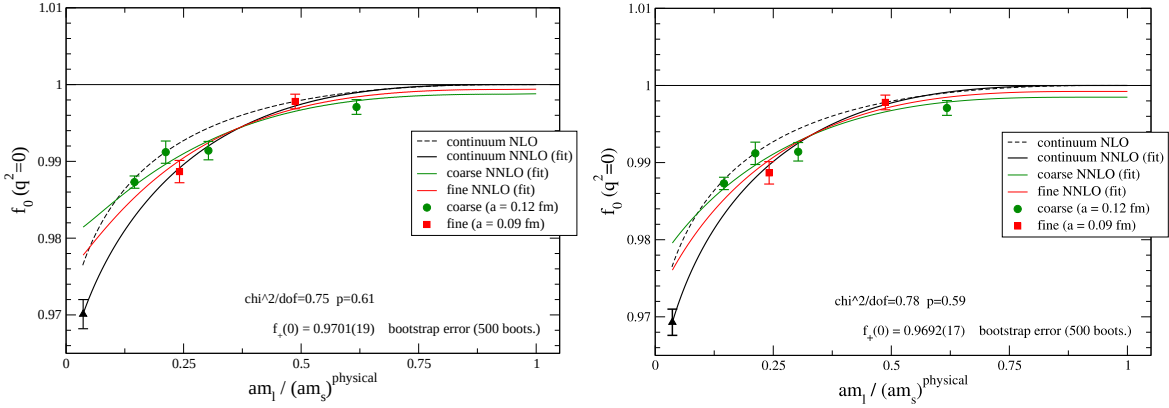


Figure 2: Left-hand plot: example of chiral-continuum extrapolations using the fit function in Eq. (2.1) with $C_6^{(a)} = 0$ and free L_i 's and priors equal to the results in Ref. [8]. Right-hand side: example using the fit function in Eq. (2.2) with $C_6^{(a)} = C_6^{(3)} = C_6^{(4)} = 0$. Errors are statistical only, from 500 bootstrap ensembles.

The setup and methodology of the calculation is common to the asqtad $N_f = 2 + 1$ calculation and is described in Sec. 1. Aside from the reduction in discretization errors provided by having HISQ sea quarks, the main improvement of this calculation respect to the asqtad $N_f = 2 + 1$ one is that we will include ensembles with physical light-quark masses. The parameters of the ensembles we plan to include in this analysis, as well as the status of the runs, are shown in Table 2. The plan is to have around 1000 configurations per ensemble and 4-5 different source-sink separations per ensemble at three different values of the lattice spacing. For the key ensembles we are generating data for 8 time sources, and, for the remaining ensembles, 4 time sources. For the light and strange valence-quark masses we will use the physical values. For the charm-quark masses, we will simulate at a value equal to the sea charm-quark mass in addition to the current estimate of the physical one, to allow for later corrections of am_c^{phys} .

$\approx a$ (fm)	am_l/am_h	am_c	Volume	N_{conf} available	$N_{sources}$	N_T	% run completed
0.15	0.035	0.831	$32^3 \times 48$	1020	8	5	100
0.12	0.200	0.635	$24^3 \times 64$	1053	4	4	100
	0.100	0.628	$32^3 \times 64$	1020	4	4	0
	0.035	0.628	$48^3 \times 64$	460	8	4	50
0.09	0.200	0.440	$32^3 \times 96$	1011	4	4	0
	0.100	0.430	$48^3 \times 96$	1000	4	4	0
	0.035	0.432	$64^3 \times 96$	497	8	4	0

Table 2: HISQ ensembles and simulation details. $N_{sources}$ is the number of time sources, and N_T the number of sink-source separations for which we have generated data. The number of configurations, N_{conf} available and the status of the runs (last column) correspond to July 2012.

In these runs we generate the correlation functions needed for the calculation of the form factor at zero momentum transfer for both $K \rightarrow \pi l \nu$ and $D \rightarrow K(\pi) l \nu$. The energies of the pions

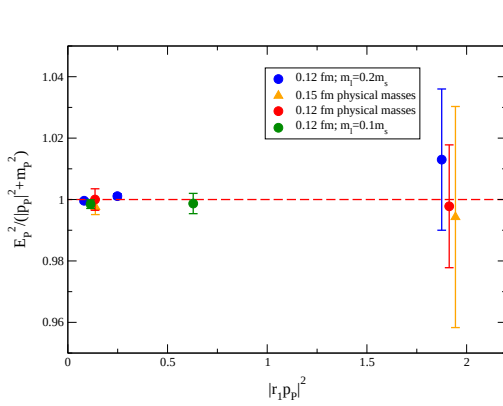


Figure 3: Deviation of our data from the continuum dispersion relation prediction.

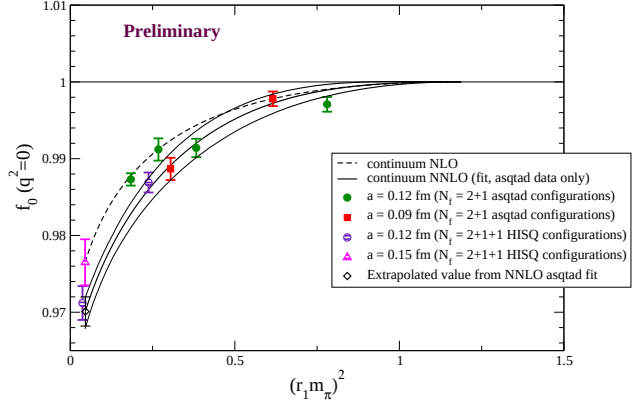


Figure 4: Form factor $f_+^{K\pi}(0)$ as a function of the π mass from the asqtad $N_f = 2 + 1$ and the HISQ $N_f = 2 + 1 + 1$ calculations, together with the results from a fit to asqtad $N_f = 2 + 1$ alone, also plotted on the left-hand side of Fig. 2.

and kaons generated on those ensembles show very little deviation from the continuum dispersion relation, see Fig. 3. The points with larger errors in that plot correspond to the energies needed to inject momentum in a K to get $q^2 = 0$ in $K \rightarrow \pi l \nu$ when we have physical light-quark masses. Thus, for physical light-quark masses, moving pions will give us significantly smaller statistical errors than moving kaons in $K \rightarrow \pi l \nu$ decays.

We fit the correlation functions generated on the HISQ configurations for the $K \rightarrow \pi l \nu$ decays using the same fitting functions and following the same strategy described in Sec. 1. The preliminary results from these fits are shown in Fig. 4, together with the data generated on the asqtad configurations and the results from the fit to the asqtad data alone (left plot in Fig. 2). The $N_f = 2 + 1 + 1$ HISQ data are very close to the continuum line obtained by fitting the $N_f = 2 + 1$ asqtad data. In particular, the point corresponding to the ensemble with physical quark masses and $a \approx 0.12$ fm lies right on top of the extrapolated value we got from the asqtad fit. This seems to indicate that the discretization effects in the HISQ data are going to be smaller than in the asqtad data, as expected. The statistical error of the physical mass point is $\sim 0.2\%$, larger than the $0.1 - 0.15\%$ error we got for larger masses, but of the same order as the extrapolated value.

4. Conclusions

We have nearly completed the calculation of $f_+^{K\pi}(0)$ at two different values of the lattice spacing using the asqtad $N_f = 2 + 1$ MILC configurations. The last step towards finishing the calculation is checking the NLO partially quenched $S\chi$ Pt expressions and completing the error budget. We estimate that the total error is going to be between $0.35 - 0.5\%$, dominated by the statistical and extrapolation errors ($0.2 - 0.3\%$) and the uncertainty associated with the deviation of am_s^{sea} from the physical value ($\sim 0.2\%$). We are also investigating the impact of subleading errors, such as finite volume effects. The total error will be competitive with current state-of-the-art calculations [10, 11].

The dominant two errors in the calculation on the asqtad $N_f = 2 + 1$ configurations will be reduced in the next step of our program namely, the calculation on the HISQ $N_f = 2 + 1 + 1$ configurations, for which we have shown preliminary results here. Having data at the physical quark masses will reduce the statistical and extrapolation errors, as well as the one associated with the choice of chiral fitting function. Discretization errors are also considerably smaller for the HISQ action than for the asqtad action, as explicitly seen in Fig. 4. Finally, the strange sea-quark masses are much better tuned on the HISQ ensembles, and we are including the effects of the dynamical charm-quark.

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References

- [1] M. Antonelli *et al.*, Eur. Phys. J. **C69**, 399-424 (2010). [arXiv:1005.2323 [hep-ph]].
- [2] V. Cirigliano, J. Jenkins and M. Gonzalez-Alonso, Nucl. Phys. B **830** (2010) 95 [arXiv:0908.1754 [hep-ph]].
- [3] H. Na, C. T. H. Davies, E. Follana, G. P. Lepage, J. Shigemitsu, Phys. Rev. **D82** (2010) 114506. [arXiv:1008.4562 [hep-lat]].
- [4] C. T. Sachrajda and G. Villadoro, Phys. Lett. B **609** (2005) 73 [hep-lat/0411033].
- [5] E. Gámiz, C. DeTar, A. X. El-Khadra, A. S. Kronfeld, P. B. Mackenzie and J. Simone, PoS(Lattice 2011)281 [arXiv:1111.2021 [hep-lat]].
- [6] J. Bijnens, P. Talavera, Nucl. Phys. **B669** (2003) 341-362. [hep-ph/0303103].
- [7] J. Bijnens, G. Colangelo and G. Ecker, JHEP **9902** (1999) 020 [hep-ph/9902437].
- [8] G. Amoros, J. Bijnens and P. Talavera, Nucl. Phys. B **602** (2001) 87 [hep-ph/0101127].
- [9] A. Bazavov *et al.* [MILC Collaboration], PoS(Lattice 2009)079 [arXiv:0910.3618 [hep-lat]].
- [10] P. A. Boyle *et al.* [RBC-UKQCD Collaboration], Eur. Phys. J. C **69** (2010) 159 [arXiv:1004.0886 [hep-lat]].
- [11] V. Lubicz *et al.* [ETM Collaboration], Phys. Rev. D **80** (2009) 111502 [arXiv:0906.4728 [hep-lat]].

Semileptonic B to D decays at nonzero recoil with 2+1 flavors of improved staggered quarks

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The Fermilab Lattice and MILC collaborations are completing a comprehensive program of heavy-light physics on MILC (2+1)-flavor asqtad ensembles with lattice spacings as small as 0.045 fm and light-to-strange-quark mass ratios as low as 1/20. We use the Fermilab interpretation of the clover action for heavy valence quarks and the asqtad action for the light valence quarks. The central goal of the program is to provide ever more exacting tests of the unitarity of the CKM matrix. We present preliminary results for one part of the program, namely the analysis of the semileptonic decay $B \rightarrow D\ell\nu$ at nonzero recoil.

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1. Introduction

The CKM matrix element $|V_{cb}|$ is a key quantity in Standard-Model tests. It normalizes the legs of the unitarity triangle. The dominant uncertainty in $|V_{cb}|$ comes from theoretical determinations of the hadronic form factors for $B \rightarrow c\ell\nu + \dots$. The exclusive processes $B \rightarrow D\ell\nu$ and $B \rightarrow D^*\ell\nu$ [1, 2, 3] can be studied in lattice gauge theory. Here we report on results for $B \rightarrow D\ell\nu$. Lattice calculations at zero recoil typically have the smallest errors. However, because of the phase space suppression near zero recoil in $B \rightarrow D\ell\nu$, experimental errors are largest there. Thus, we aim to work at nonzero recoil where the combined experimental and theoretical error is minimized. This work updates our previous report [4] with all ensembles now included in the analysis.

The differential decay rate $d\Gamma(B \rightarrow D\ell\bar{\nu})/dq^2$ is, for $m_\ell^2 \ll \min(M_B^2, q^2)$, proportional to $|f_+|^2$ for $\ell = e, \mu$, where for $q = p_B - p_D$,

$$\langle D(p_D) | \mathcal{V}^\mu | B(p_B) \rangle = f_+(q^2) \left[(p_B + p_D)^\mu - \frac{M_B^2 - M_D^2}{q^2} q^\mu \right] + f_0(q^2) \frac{M_B^2 - M_D^2}{q^2} q^\mu. \quad (1.1)$$

Here $\mathcal{V}^\mu = \bar{b}\gamma^\mu c$ is the $b \rightarrow c$ vector current and f_+ and f_0 are the vector and scalar form factors, respectively. The alternative form factors h_+ and h_- are convenient:

$$\frac{\langle D(p_D) | \mathcal{V}^\mu | B(p_B) \rangle}{\sqrt{M_B M_D}} = h_+(w)(v + v')^\mu + h_-(w)(v - v')^\mu, \quad (1.2)$$

where $v = p_B/M_B$ and $v' = p_D/M_D$. They are related to f_+ and f_0 through

$$\begin{aligned} f_+(q^2) &= \frac{1}{2\sqrt{r}} [(1+r)h_+(w) - (1-r)h_-(w)], \\ f_0(q^2) &= \sqrt{r} \left[\frac{w+1}{1+r} h_+(w) - \frac{w-1}{1-r} h_-(w) \right], \end{aligned} \quad (1.3)$$

where $r = M_D/M_B$ and $q^2 = M_B^2 + M_D^2 - 2wM_B M_D$ or $w = v \cdot v'$.

2. Lattice-QCD calculation

We are carrying out calculations on 14 lattice ensembles generated in the presence of $2+1$ flavors of improved (asqtad) staggered sea quarks [7] with light-quark masses and lattice spacings shown in Fig. 1.

In the B meson rest frame for any recoil D -momentum $\mathbf{p}$ we can obtain h_+ and h_- from matrix elements of the current starting from ratios of lattice matrix elements R_+ and R_- , and x_f , where

$$\begin{aligned} R_+(\mathbf{p}) &\equiv \frac{\langle D(\mathbf{p}) | V^4 | B(\mathbf{0}) \rangle}{\langle D(\mathbf{p}) | V^1 | B(\mathbf{0}) \rangle} \\ R_-(\mathbf{p}) &\equiv \frac{\langle D(\mathbf{p}) | V^1 | B(\mathbf{0}) \rangle}{\langle D(\mathbf{p}) | V^4 | B(\mathbf{0}) \rangle} \\ x_f(\mathbf{p}) &\equiv \frac{\langle D(\mathbf{p}) | V^1 | D(\mathbf{0}) \rangle}{\langle D(\mathbf{p}) | V^4 | D(\mathbf{0}) \rangle} \\ w(\mathbf{p}) &= [1 + x_f(\mathbf{p})^2] / [1 - x_f(\mathbf{p})^2] \\ h_+(w) &= R_+(\mathbf{p}) [1 - x_f(\mathbf{p}) R_-(\mathbf{p})] \\ h_-(w) &= R_+(\mathbf{p}) [1 - R_-(\mathbf{p}) / x_f(\mathbf{p})]. \end{aligned} \quad (2.1)$$

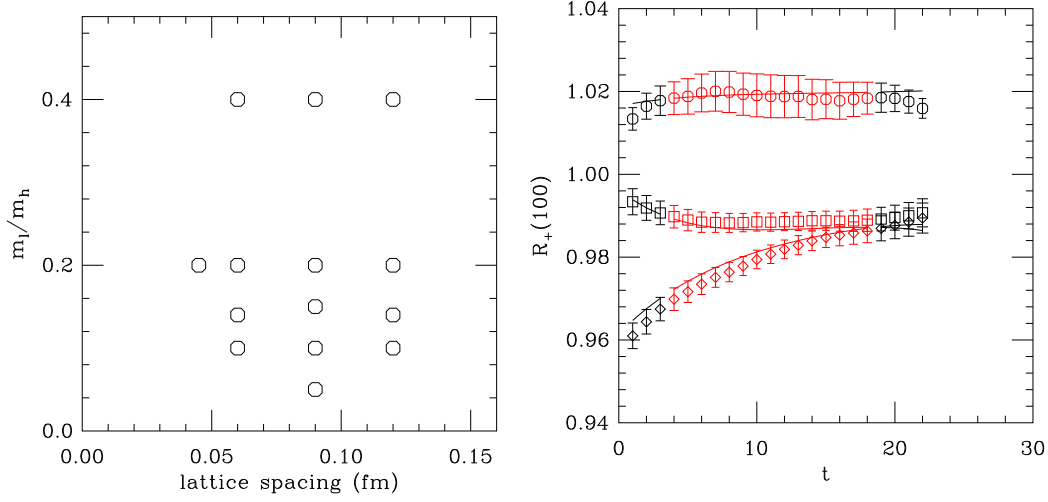


Figure 1: Left panel: parameters of the 14 lattice ensembles in this study. Plotted are values of the light to strange sea quark mass ratio m_ℓ/m_h vs. the approximate lattice spacing in fm. Right panel: example from the $a = 0.06$ fm, $m_\ell/m_h = 0.15$ ensemble with $T = 24, 25$. Upper curve: the zero-recoil double ratio, middle curve: the ratio $R_+(\mathbf{p}, t)/R_+(\mathbf{0}, t)$ for the 1S smeared D -meson interpolator, and bottom curve: the local interpolator. Red points are included in the fit ($p = 0.15$).

At zero recoil, we can also use the double ratio of Hashimoto *et al* [5]:

$$|h_+(\mathbf{0})|^2 = \frac{\langle D(\mathbf{0})|V^1|B(\mathbf{0})\rangle \langle B(\mathbf{0})|V^1|D(\mathbf{0})\rangle}{\langle D(\mathbf{0})|V^4|D(\mathbf{0})\rangle \langle B(\mathbf{0})|V^4|B(\mathbf{0})\rangle}. \quad (2.2)$$

The continuum $\mathcal{V}^\mu$ and lattice V^μ currents are matched through $\mathcal{V}_{cb}^\mu = Z_{V_{cb}^\mu} V_{cb}^\mu$. We use a mostly nonperturbative method [5], writing

$$Z_{V_{cb}^\mu} = \rho_{V_{cb}^\mu} \sqrt{Z_{V_{cc}^4} Z_{V_{bb}^4}}, \quad (2.3)$$

and determine $\rho_{V_{cb}^\mu}$ from one-loop lattice perturbation theory.

In addition to the two-point functions, we need matrix elements $\langle Y(\mathbf{p})|V^\mu|X(0)\rangle$ for $X, Y \in \{B, D\}$. They are constructed from naive light spectator quark propagators and clover heavy quark propagators in the Fermilab interpretation [6] as shown in Fig. 2. Valence bottom and charm quark masses were tuned to the “kinetic” B_s and D_s masses. The mass of the naive light spectator quark is set equal to that of the light sea quark.

For interpolating operators $\mathcal{O}_X$, we compute two-point and three-point functions

$$C^{2pt,X}(\mathbf{p}, t) = \langle \mathcal{O}_X^\dagger(0) \mathcal{O}_X(t) \rangle, \quad (2.4)$$

$$C^{3pt,X \rightarrow Y,\mu}(\mathbf{p}; 0, t, T) = \langle \mathcal{O}_Y^\dagger(0) V^\mu(t) \mathcal{O}_X(T) \rangle. \quad (2.5)$$

We use both point and 1S smeared interpolating operators for the D meson and 1S smeared interpolating operators for the B .

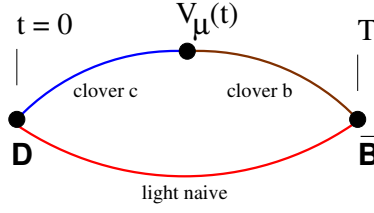


Figure 2: Valence quark line diagram for $B \rightarrow D$.

2.1 Two-point and three-point correlator fits

We obtain the lattice form factors via a two-step procedure. First, we fit the B - and D -meson two-point correlators to obtain the energies and overlap factors. Then we use these determinations as constraints (with Bayesian priors) in the three-point fits. For illustration, we show the reduction of the three-point and two-point functions to obtain $R_+(p) = \langle D(\mathbf{p}) | V^4 | B(\mathbf{0}) \rangle$. We include excited B and D contributions indicated with a prime but not both together:

$$\begin{aligned} C_{V^4}^{3pt, B \rightarrow D}(\mathbf{p}, t) &= \sqrt{Z_D(\mathbf{p})} \frac{e^{-E_D t}}{\sqrt{2E_D}} \langle D(\mathbf{p}) | V^4 | B(\mathbf{0}) \rangle \frac{e^{-m_B(T-t)}}{\sqrt{2m_B}} \sqrt{Z_B(\mathbf{0})} \\ &+ \sqrt{Z_{D'}(\mathbf{p})} \frac{e^{-E_{D'} t}}{\sqrt{2E_{D'}}} \langle D'(\mathbf{p}) | V^4 | B(\mathbf{0}) \rangle \frac{e^{-m_B(T-t)}}{\sqrt{2m_B}} \sqrt{Z_B(\mathbf{0})} \\ &+ \sqrt{Z_D(\mathbf{p})} \frac{e^{-E_D t}}{\sqrt{2E_D}} \langle D(\mathbf{p}) | V^4 | B'(\mathbf{p}) \rangle \frac{e^{-m_{B'}(T-t)}}{\sqrt{2m_{B'}}} \sqrt{Z_{B'}(\mathbf{0})}, \end{aligned} \quad (2.6)$$

or

$$C_{V^4}^{3pt, B \rightarrow D}(\mathbf{p}, t) = C_0(\mathbf{p}) \langle D(\mathbf{p}) | V^4 | B(\mathbf{0}) \rangle e^{-E_D t} e^{-m_B(T-t)} \left[1 + C_1(\mathbf{p}) e^{-\Delta E_D t} + C_2(\mathbf{p}) e^{(t-T)\Delta m_B} \right], \quad (2.7)$$

where $C_0(\mathbf{p})$, $\Delta E_D = E_{D'} - E_D$, and $\Delta m_B = m_{B'} - m_B$ come from fits to two-point correlators. Terms oscillating as $(-)^t$ (not shown) are introduced by the naive light quark. We suppress their contributions by averaging over T , $T+1$ and t , $t+1$, as introduced in [1].

Putting information from three- and two-point functions together, we get

$$\begin{aligned} R_+(\mathbf{p}, t) &\equiv \frac{C_{V^4}^{3pt, B \rightarrow D}(\mathbf{p}, t) e^{(E_D - m_B)t + (m_B - m_D)T/2}}{\sqrt{C_{V^4}^{3pt, D \rightarrow D}(\mathbf{0}, t) C_{V^4}^{3pt, B \rightarrow B}(\mathbf{0}, t)}} \sqrt{\frac{Z_D(\mathbf{0}) E_D}{Z_D(\mathbf{p}) m_D}} \\ &\approx R_+(\mathbf{p}) \left[1 + s_1(\mathbf{p}) e^{-\Delta E_D t} + s_2(\mathbf{p}) e^{(t-T)\Delta m_B} \right]. \end{aligned} \quad (2.8)$$

The zero-recoil form factor $h_+(\mathbf{0}) = R_+(\mathbf{0})$ can be calculated very accurately from the double ratio. A good strategy is to use it to normalize the nonzero recoil values:

$$\frac{R_+(\mathbf{p}, t)}{R_+(\mathbf{0}, t)} = \frac{R_+(\mathbf{p})}{R_+(\mathbf{0})} \exp(\delta m t) + A(\mathbf{p}) \exp(-\Delta E_D t) + B(\mathbf{p}) \exp(\Delta m_B t), \quad (2.9)$$

where $\delta m = 0$, $\Delta E_D = E_{D'} - E_D$, and $\Delta m_B = m_{B'} - m_B$ are constrained by fits to two-point functions.

We do a simultaneous fit to three three-point functions, as illustrated in the right panel of Fig. 1 and determine R_+ , R_- , and x_f for each momentum (recoil parameter w), from which we determine h_+ and h_- .

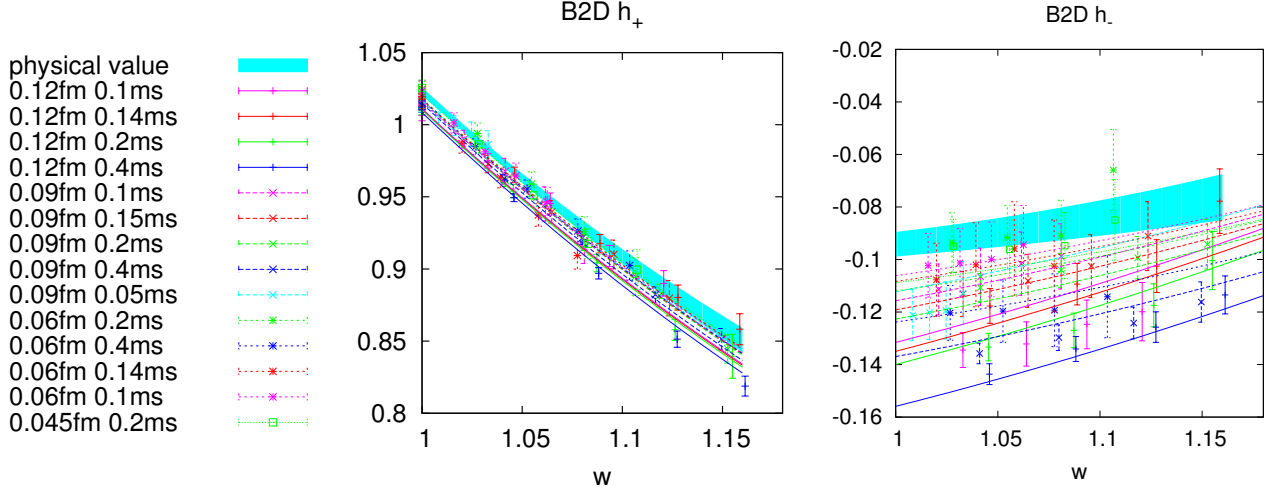


Figure 3: Form factors h_+ (left) and h_- (right) as a function of the recoil parameter w . The curves in each panel are a result of a simultaneous fit to the chiral-continuum expressions of Eq. (2.10) with $p = 0.68$ for the h_+ fit and $p = 0.41$ for the h_- fit.

2.2 Chiral-continuum extrapolation and q^2 parameterization

The resulting form factors h_+ and h_- are shown in Fig. 3. We fit them to the expressions

$$\begin{aligned}
 h_+(a, m_\ell, w) &= 1 - \rho_+^2(w-1) + k_+(w-1)^2 + \frac{X_+(\Lambda_\chi)}{m_c^2} + c_{1,+}m_\ell + c_{a,+}a^2 + c_{a,w,+}a^2(w-1) \\
 &\quad + \frac{g_{D^*D\pi}^2}{16\pi^2 f^2} \log_{1-\text{loop}}(\Lambda_\chi, w, m_\ell, a) \\
 h_-(a, m_\ell, w) &= \frac{X_-}{m_c} - \rho_-^2(w-1) + k_-(w-1)^2 + c_{1,-}m_\ell + c_{a,-}a^2 + c_{a,w,-}a^2(w-1)
 \end{aligned} \tag{2.10}$$

for light spectator quark mass m_ℓ , lattice spacing a , and $w = v \cdot v'$. For the one-loop chiral logs we use a staggered fermion version of Chow and Wise [9]. Thus, these fit functions contain the correct next-to-leading-order chiral perturbation theory expressions, including staggered discretization effects [10]. As can be seen, the dependence of h_+ on a and m_ℓ/m_h is quite mild. We expect h_- to have larger discretization effects than h_+ because of different HQET power counting. This is consistent with what we see in the data. For $|V_{cb}|$, the contribution coming from h_- over the entire kinematic range is small, so the larger errors in h_- don't increase the overall error much. These features with 14 ensembles are consistent with our previous findings with four ensembles [10].

To compare the lattice and experimental form factors we need to extrapolate to larger w (equivalently q^2). We do this using the z -expansion of Boyd, Grinstein and Lebed [11], which provides a model-independent parameterization of the q^2 dependence of f_+ and f_0 . This expansion builds in constraints from analyticity and unitarity. It is based on the conformal map

$$z(w) = \frac{\sqrt{1+w} - \sqrt{2}}{\sqrt{1+w} + \sqrt{2}}, \tag{2.11}$$

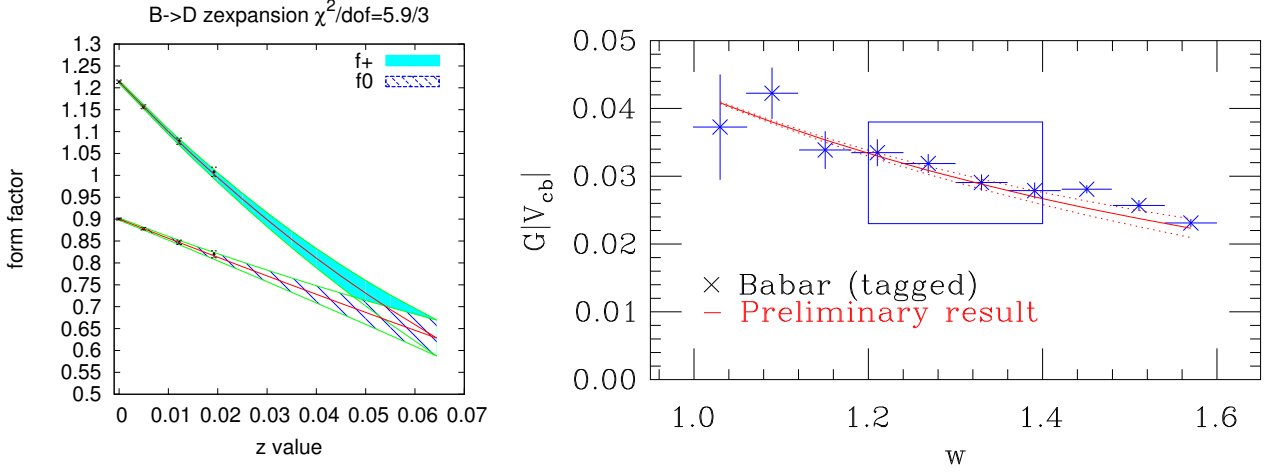


Figure 4: Left: form factors f_+ and f_0 parameterized by the z expansion ($p = 0.12$). Right: comparison with experimental results from the Babar collaboration [12]. The red line gives our result. The red dotted lines show only statistical errors. The boxed region appears to have the smallest combined error.

which maps the physical region $w \in [1, 1.59]$ to $z \in [0, 0.0644]$. It pushes poles and branch cuts far away at $|z| \approx 1$. Form factors are then parameterized as

$$f_i(z) = \frac{1}{P_i(z)\phi_i(z)} \sum_{n=0}^{\infty} a_{i,n} z^n, \quad (2.12)$$

where $P_i(z)$ are the Blaschke factors and ϕ_i are the “outer functions”. The latter are chosen to simplify the unitarity bound:

$$\sum_n |a_{i,n}|^2 \leq 1. \quad (2.13)$$

In practice, we need only the first few coefficients in the expansion. We also impose the kinematic constraint $f_+ = f_0$ at $q^2 = 0$ or $z \approx 0.0644$.

To implement the z expansion, we start from the value of f_+ and f_0 at the physical point, as determined from the chiral/continuum fit. We choose four w values, $w = 1.00, 1.04, 1.10$, and 1.16 , and use the corresponding form factor values to determine the coefficients $a_{i,0}$, $a_{i,1}$, and $a_{i,2}$. These, then, are used to parameterize the form factors over the full kinematic range, as shown in the left panel of Fig. 4.

We compare our result with experimental measurements from the Babar collaboration [12] in Fig. 4. For present purposes we take $|V_{cb}|$ from $B \rightarrow D^* \ell \nu$ at zero recoil [3].

3. Future plans

To complete the analysis, we need to apply small corrections resulting from adjusting the charm and bottom quark masses to their tuned values, implement the full current renormalization, and compile a complete error budget.

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References

- [1] C. Bernard *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. **D79** 014506 (2009). [[arXiv:0808.2519 \[hep-lat\]](#)].
- [2] J. Laiho, R. S. Van de Water, Phys. Rev. **D73**, 054501 (2006). [[hep-lat/0512007](#)].
- [3] J. A. Bailey *et al.* [Fermilab Lattice and MILC Collaborations], *PoS(Lattice 2010)* 311 (2010) [[arXiv:1011.2166 \[hep-lat\]](#)].
- [4] Si-Wei Qiu *et al.* [Fermilab Lattice and MILC Collaborations], *PoS(Lattice 2011)* 289 (2011) [[arXiv:1111.0677 \[hep-lat\]](#)].
- [5] S. Hashimoto, A. S. Kronfeld, P. B. Mackenzie, S. M. Ryan, and J. N. Simone, Phys. Rev. **D66**, 014503 (2002). [[hep-ph/0110253](#)]; J. Harada, S. Hashimoto, A. S. Kronfeld, and T. Onogi, Phys. Rev. D **65**, 094514 (2002) [[hep-lat/0112045](#)].
- [6] A. X. El-Khadra, A. S. Kronfeld, P. B. Mackenzie, Phys. Rev. **D55**, 3933-3957 (1997). [[hep-lat/9604004](#)].
- [7] T. Blum *et al.* [MILC Collaboration], Phys. Rev. D **55**, 1133 (1997) [[hep-lat/9609036](#)].
C. W. Bernard *et al.* [MILC Collaboration], Phys. Rev. D **58**, 014503 (1998) [[hep-lat/9712010](#)].
K. Orginos *et al.* [MILC Collaboration], Phys. Rev. D **59**, 014501 (1999) [[hep-lat/9805009](#)].
J. F. Lagaë and D. K. Sinclair, Phys. Rev. D **59**, 014511 (1999) [[hep-lat/9806014](#)]. G. P. Lepage, Phys. Rev. D **59**, 074502 (1999) [[hep-lat/9809157](#)]. K. Orginos *et al.* [MILC Collaboration], Phys. Rev. D **60**, 054503 (1999) [[hep-lat/9903032](#)].
- [8] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010) [[arXiv:0903.3598 \[hep-lat\]](#)].
- [9] C. K. Chow and M. B. Wise, Phys. Rev. D **48** (1993) 5202 [[arXiv:hep-ph/9305229](#)].
- [10] J. A. Bailey *et al.*, Phys. Rev. D **85**, 114502 (2012) [Erratum-ibid. D **86**, 039904 (2012)] [[arXiv:1202.6346 \[hep-lat\]](#)].
- [11] C. G. Boyd, B. Grinstein and R. F. Lebed, Phys. Rev. Lett. **74**, 4603 (1995) [[hep-ph/9412324](#)].
- [12] B. Aubert *et al.* [BABAR Collaboration], Phys. Rev. Lett. **104**, 011802 (2010) [[arXiv:0904.4063 \[hep-ex\]](#)].

Charmonium mass splittings at the physical point

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We present results from an ongoing study of mass splittings of the lowest lying states in the charmonium system. We use clover valence charm quarks in the Fermilab interpretation, an improved staggered (asqtad) action for sea quarks, and the one-loop, tadpole-improved gauge action for gluons. This study includes five lattice spacings, 0.15, 0.12, 0.09, 0.06, and 0.045 fm, with two sets of degenerate up- and down-quark masses for most spacings. We use an enlarged set of interpolation operators and a variational analysis that permits study of various low-lying excited states. The masses of the sea quarks and charm valence quark are adjusted to their physical values. This large set of gauge configurations allows us to extrapolate results to the continuum physical point and test the methodology.

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Table 1: Parameters of the ensembles used in this study. Simulation light and heavy bare sea quark masses are denoted m_l and m_h . Mass-independent, tuned physical bare masses are denoted $\hat{m}$ for degenerate up and down quarks and m_s for strange. Also shown are the approximate lattice spacing, the lattice size, and the number of source times used (typically four per gauge configuration).

$\approx a(\text{fm})$	am_l	am_h	$a\hat{m}$	am_s	size	sources
0.15	0.0097	0.0484	0.0015180	0.04213	$16^3 \times 48$	2484
0.15	0.0048	0.0484	0.0015180	0.04213	$20^3 \times 48$	2416
0.12	0.01	0.050	0.0012150	0.03357	$20^3 \times 64$	4036
0.12	0.005	0.050	0.0012150	0.03357	$24^3 \times 64$	3328
0.09	0.0062	0.031	0.0008923	0.02446	$28^3 \times 96$	3728
0.09	0.0031	0.031	0.0009004	0.02468	$40^3 \times 96$	4060
0.06	0.0036	0.018	0.0006401	0.01751	$48^3 \times 144$	2604
0.06	0.0018	0.018	0.0006456	0.01766	$64^3 \times 144$	1984
0.045	0.0024	0.014	0.0004742	0.01298	$64^3 \times 192$	3204

1. Objectives

The wealth of excited charmonium states discovered at the B factories presents a challenge for interpretation (and, in some cases, confirmation). Some states could be spin-exotic hybrids and some “molecular” states. In principle, lattice QCD should provide a reliable guide to the interpretation of these states [1, 2, 3, 4, 5, 6]. For levels above the open charm threshold, the treatment of multihadronic scattering states presents a technical challenge. Other challenges are controlling heavy-quark discretization errors and, for some levels, including annihilation effects. Matching theory to experiment requires a relatively high degree of precision.

In the present study our more limited objective is to lay the foundation for future work by carrying out a high-precision study of the splittings of the low-lying states. Here we use clover charm quarks in the Fermilab interpretation [7]. To the extent we can reproduce the known splittings, we test the methodology. Validation of the method also gives confidence in other studies that use the same fermion formulations.

This work expands and extends our previous study [1] with clover (Fermilab) quarks and 2+1 flavors of asqtad sea quarks. We use a large variational basis of interpolating operators, and we extrapolate to zero lattice spacing and physical sea-quark masses.

2. Methodology

2.1 Gauge-field ensembles

We work with a large set of gauge-field ensembles generated in the presence of 2+1 flavors of asqtad sea quarks and a 1-loop tadpole improved gauge field [8, 9]. Parameters are listed in Table 1. These tuned values for the light quark masses are determined from chiral fits to masses and decay constants of the light pseudoscalar mesons [9].

Table 2: Examples of charmonium interpolating operators used in this study. Here operators for the T_1^{PC} irrep are shown. In the notation below, ∇_i generates a discrete covariant difference in direction i , $\mathbb{D}_k = |\varepsilon_{ijk}| \nabla_i \nabla_j$, and $\mathbb{B}_i = \varepsilon_{ijk} \nabla_i \nabla_j$.

T_1^{--}	T_1^{+-}	T_1^{-+}	T_1^{++}
γ_i	$\gamma_4 \gamma_5 \gamma_i$	$\gamma_4 \nabla_i$	$\gamma_5 \gamma_i$
$\gamma_4 \gamma_i$	$\gamma_5 \nabla_i$	$\varepsilon_{ijk} \gamma_4 \gamma_5 \gamma_j \nabla_k$	$\varepsilon_{ijk} \gamma_j \nabla_k$
∇_i	$\gamma_4 \gamma_5 \nabla_i$	$\varepsilon_{ijk} \gamma_j \mathbb{B}_k$	$\varepsilon_{ijk} \gamma_4 \gamma_j \nabla_k$
$\varepsilon_{ijk} \gamma_5 \gamma_j \nabla_k$	$ \varepsilon_{ijk} \gamma_4 \gamma_5 \gamma_j \mathbb{D}_k$	$\varepsilon_{ijk} \gamma_4 \gamma_j \mathbb{B}_k$	$ \varepsilon_{ijk} \gamma_5 \gamma_j \mathbb{D}_k$
$ \varepsilon_{ijk} \gamma_j \mathbb{D}_k$	$\mathbb{B}_i$		$\gamma_4 \mathbb{B}_i$
$ \varepsilon_{ijk} \gamma_4 \gamma_j \mathbb{D}_k$	—		$\varepsilon_{ijk} \gamma_4 \gamma_5 \gamma_j \mathbb{B}_k$
$\gamma_5 \mathbb{B}_i$			
$\gamma_4 \gamma_5 \mathbb{B}_i$			

2.2 Interpolating operators

As mentioned above, we use clover charm quarks with the Fermilab interpretation. Interpolating operators are classified according to their cubic group irreps and their P and C quantum numbers. We use a large basis of operators following Liao and Manke [10] and the JLab group [11]. Our operators are constructed from stochastic wall sources. Averaging over stochastic sources results in both local and smeared bilinears of the form

$$\mathcal{O}_i(x) = \bar{q}(x) O_i q(x) \quad \mathcal{O}'_i(x) = \bar{q}(x) O_i S q(x), \quad (2.1)$$

where O_i is one of several operators, as illustrated in Table 2, and S represents covariant Laplacian smearing. (Only one width of smearing is included.) We *do not* include, however, any explicit open charm or charmonium/light-meson states in the list.

2.3 Variational determination of energy levels

In each channel (defined by the cubic group irrep and P and C), we use the standard variational methodology [12, 13] for determining the lowest lying states. For interpolating operators O_i , we define the correlation matrix

$$C_{ij}(t) = \langle O_i(t) O_j(0) \rangle. \quad (2.2)$$

The goal is to determine, to good approximation, the energies E_n in the spectral decomposition

$$C_{ij}(t) = \sum_n z_{in} z_{jn}^* \frac{\exp(-E_n t)}{2E_n}. \quad (2.3)$$

Ideally, the eigenvalues of the transfer matrix T^{t-t_0} from time t_0 to time t are $\lambda_n(t, t_0) = \exp[-E_n(t - t_0)]$. With a finite set of interpolating operators and a truncated list of energies, the eigenvalues receive contributions from higher states, which are modeled with [11]

$$\lambda_n(t, t_0) = a_0 \exp[-E_n(t - t_0)] + a_1 \exp[-E'_n(t - t_0)] + \dots \quad (2.4)$$

The lowest energy E_n for each n becomes an estimate of the n th excited state in that channel.

2.4 Scale and charm quark mass

The lattice scale is based on the Sommer r_1 parameter. It is determined in two steps. First, we have detailed measurements of its value in lattice units, r_1/a , from the heavy-quark potential. Then, r_1 itself is determined on the same lattice ensembles from a mass-independent, partially quenched, staggered χ PT analysis of the light pseudoscalar masses and decay constants. That analysis used f_π , M_π , and M_K to determine the physical bare light quark masses $\hat{m}$ and m_s and $r_1 = 0.3117(22)$ fm [14].

Once the lattice scale is known, we tune the charm quark mass by requiring that the kinetic mass M_2 of the D_s meson, defined through the dispersion relation,

$$E_{D_s}(\mathbf{p}) = M_1 + \mathbf{p}^2/(2M_2) + \dots, \quad (2.5)$$

matches the experimental value. In our implementation of the Fermilab method, we do not tune the value of M_1 , the rest mass, however. Thus, the rest mass of the quark suffers from substantial discretization artifacts (except when $am_c \ll 1$). This contribution cancels, however, in the difference of two hadron rest masses. For that reason we report only level splittings below, e.g., $M_1(2S) - M_1(1S)$. For further discussion of this point, see Refs. [1, 7].

2.5 Sea-quark mass effects and continuum fit model

Although our gauge-field ensembles were generated in the presence of $2 + 1$ flavors of light sea quarks with fixed ratios of the bare quark masses, the initial estimate that set the simulation strange sea-quark mass was imprecise. In the worst case, on the 0.12 fm ensembles the strange sea quark was some 50% heavier than our best current estimate of its physical value in a mass-independent scheme (see Table 1). Thus, to extrapolate any of our measurements to the physical point, we include terms that model the dependence of the meson masses on sea-quark masses:

$$M = M_0 + c_1(2x_\ell + x_h) + c_2a^2, \quad (2.6)$$

where, in the notation of Table 1, $x_\ell = (m_l - \hat{m})/m_s$ and $x_h = (m_h - m_s)/m_s$.

3. Results

1S hyperfine splitting The hyperfine splitting of the 1S level provides a demanding test of the methodology [16]. The extrapolated result shown in Fig. 1 is compared with the current PDG value and the recent BESIII value[15]. Annihilation effects, which would decrease the splitting slightly [17] have not been included. The extrapolated error is ± 2 MeV and appears to favor the BESIII value. The largest contribution to the uncertainty comes from our imperfect knowledge of r_1 . In the determination of the hyperfine splitting, this uncertainty enters twice, first in setting the charm quark mass, and second, in comparing the splitting with the experimental value. In this quantity the error is amplified, not cancelled.

1P – 1S splitting Results for the spin-averaged 1P – 1S splitting are shown in Fig. 1. The error at the physical point (including the scale error) is ± 4 MeV (1%).

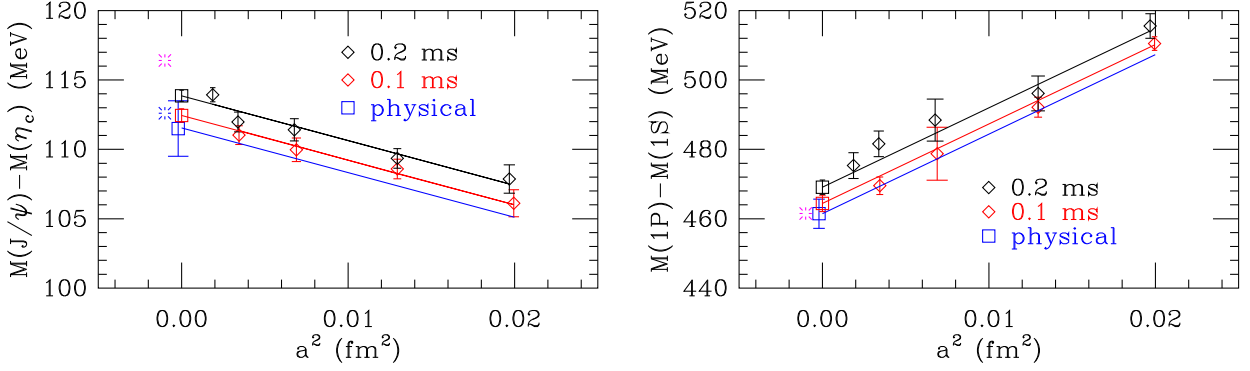


Figure 1: Left panel: $1S$ hyperfine splitting. Right panel: spin-averaged $1P - 1S$ splitting. Errors on data points are statistical only. The blue square is the physical value including the r_1 scale error. The magenta burst (slightly displaced) is the PDG value. The blue burst is the recent BESIII result [15].

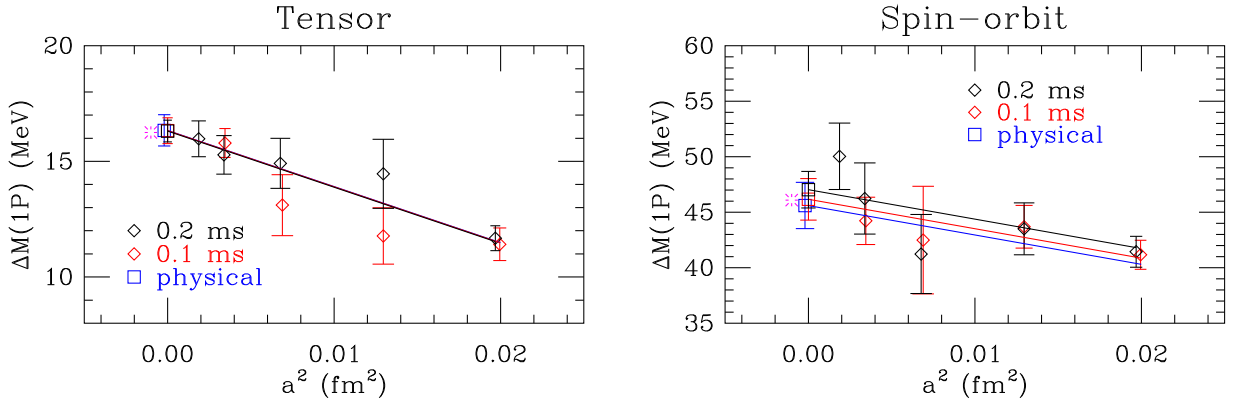


Figure 2: Left panel: $1P$ tensor mass combination. Right panel: $1P$ spin-orbit mass combination

$1P$ tensor and spin-orbit mass combinations The left panel of Fig. 2 shows the tensor mass combination

$$\frac{1}{9}[3M(\chi_{c1}) - M(\chi_{c2}) - 2M(\chi_{c0})]$$

(extrapolated error ± 0.7 MeV), and the right panel, the spin-orbit mass combination

$$\frac{1}{9}[5M(\chi_{c2}) - 2M(\chi_{c0}) - 3M(\chi_{c1})]$$

(extrapolated error ± 2 MeV). In a heavy-quark expansion these mass splittings arise from the tensor and spin-orbit terms in the effective heavy-quark potential (quark model). These results are sensitive to discretization errors arising from those terms.

$2S$ states We overestimate considerably the splitting of the $2S$ and $1S$ levels, as shown in the left panel of Fig. 3. We get 675 ± 6 MeV compared with the experimental value 606 MeV. The

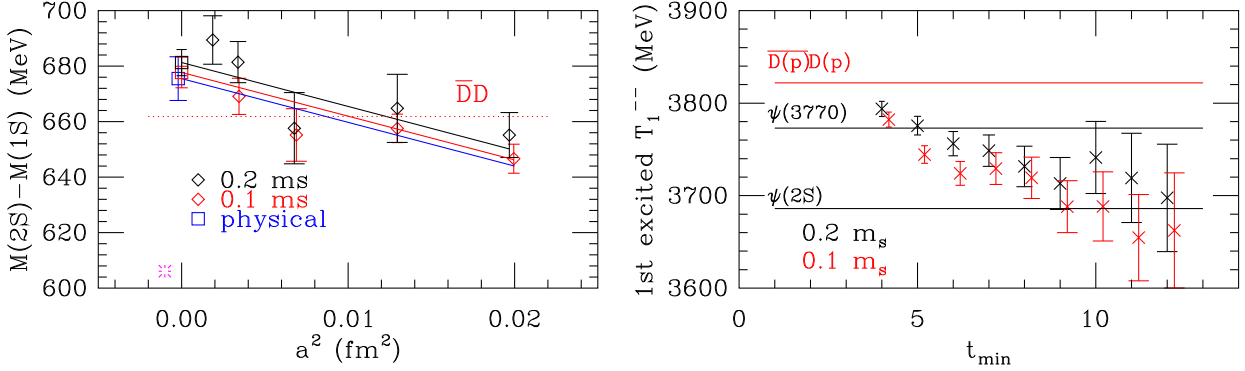


Figure 3: Left panel: Spin-averaged $2S - 1S$ splittings. Note the experimental value (magenta burst) at the lower left. The physical open charm threshold is also shown. Right panel: $\psi(2S)$ level as a function of $t_{\min}$ at $a \approx 0.09$ fm. The full energy was reconstructed by adding the measured splitting to the experimental spin-averaged $1S$ level.

same problem was seen in [1] but with less clarity. Since the $2S$ levels are close to the open charm threshold, one may speculate that by not including an explicit open charm term in the variational mix, we cannot get a good representation of these states [18]. In support of this hypothesis, in the right panel of Fig. 3, we note that the splitting of the $\psi(2S)$ level from the $1S$ ground state shows a decreasing trend as $t_{\min}$, the minimum of the fit range in $\lambda_n(t)$, is increased. Indeed, if we set a higher $t_{\min}$ value for all lattice spacings and repeat the analysis, we get 651(12) MeV. Such behavior would result if a substantial open charm component is required but the transfer matrix has only a very weak mixing between closed and open charm. Such weak mixing has been known from string-breaking studies of the static potential [19, 20].

4. Conclusions and Outlook

We can reproduce the splittings of the lowest-lying charmonium levels to a precision of a couple of MeV. At this level of precision, however, we fail to reproduce the $2S$ - $1S$ spin-averaged splitting with our set of interpolators. To complete the analysis we will develop a complete error budget. We will next try adding explicit open charm to the variational mix. We plan, also, to study bottomonium.

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References

- [1] T. Burch *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. D **81**, 034508 (2010) [[arXiv:0912.2701](#) [[hep-lat](#)]].
- [2] G. Bali, S. Collins, S. Dürr, Z. Fodor, R. Horsley, C. Hoelbling, S. D. Katz and I. Kanamori *et al.*, [[arXiv:1108.6147](#) [[hep-lat](#)]].
- [3] L. Liu, S. M. Ryan, M. Peardon, G. Moir and P. Vilaseca, [[arXiv:1112.1358](#) [[hep-lat](#)]].
- [4] Y. Namekawa *et al.* [PACS-CS Collaboration], Phys. Rev. D **84**, 074505 (2011) [[arXiv:1104.4600](#) [[hep-lat](#)]].
- [5] L. Liu, G. Moir, M. Peardon, S. M. Ryan, C. E. Thomas, P. Vilaseca, J. J. Dudek and R. G. Edwards *et al.*, [[arXiv:1204.5425](#) [[hep-ph](#)]].
- [6] D. Mohler, S. Prelovsek and R. M. Woloshyn, [[arXiv:1208.4059](#) [[hep-lat](#)]].
- [7] A. X. El-Khadra, A. S. Kronfeld and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997) [[arXiv:hep-lat/9604004](#)].
- [8] T. Blum *et al.* [MILC Collaboration], Phys. Rev. D **55**, 1133 (1997) [[hep-lat/9609036](#)].
C. W. Bernard *et al.* [MILC Collaboration], Phys. Rev. D **58**, 014503 (1998) [[hep-lat/9712010](#)].
K. Orginos *et al.* [MILC Collaboration], Phys. Rev. D **59**, 014501 (1999) [[hep-lat/9805009](#)].
J. F. Lagae and D. K. Sinclair, Phys. Rev. D **59**, 014511 (1999) [[hep-lat/9806014](#)]. G. P. Lepage, Phys. Rev. D **59**, 074502 (1999) [[hep-lat/9809157](#)]. K. Orginos *et al.* [MILC Collaboration], Phys. Rev. D **60**, 054503 (1999) [[hep-lat/9903032](#)].
- [9] A. Bazavov *et al.*, Rev. Mod. Phys. **82**, 1349 (2010) [[arXiv:0903.3598](#) [[hep-lat](#)]].
- [10] X. Liao and T. Manke, [hep-lat/0210030](#) (2002).
- [11] J. J. Dudek, R. G. Edwards, N. Mathur and D. G. Richards, Phys. Rev. D **77**, 034501 (2008) [[arXiv:0707.4162](#) [[hep-lat](#)]].
- [12] C. Michael, Nucl. Phys. B **259**, 58 (1985).
- [13] M. Lüscher and U. Wolff, Nucl. Phys. B **339**, 222 (1990).
- [14] A. Bazavov *et al.* [Fermilab Lattice and MILC Collaborations], Phys. Rev. D **85**, 114506 (2012) [[arXiv:1112.3051](#) [[hep-lat](#)]].
- [15] M. Ablikim *et al.* [BESIII Collaboration], Phys. Rev. Lett. **108**, 222002 (2012) [[arXiv:1111.0398](#) [[hep-ex](#)]].
- [16] E. Follana (HPQCD Collaboration), [PoS\(Lattice 2010\)305](#) (2010).
- [17] L. Levkova and C. DeTar, Phys. Rev. D **83**, 074504 (2011) [[arXiv:1012.1837](#) [[hep-lat](#)]].
- [18] G. S. Bali, S. Collins and C. Ehmman, Phys. Rev. D **84**, 094506 (2011) [[arXiv:1110.2381](#) [[hep-lat](#)]].
- [19] P. Pennanen *et al.* [UKQCD Collaboration], [[hep-lat/0001015](#)].
- [20] C. W. Bernard *et al.* [MILC Collaboration], Phys. Rev. D **64**, 074509 (2001) [[hep-lat/0103012](#)].