Testing the Standard Model and Fundamental Symmetries in Nuclear Physics with Lattice QCD and Effective Field Theory

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1 Research Progress

1.1 Overview

The research supported by this grant is aimed at probing the limits of the Standard Model through precision low-energy nuclear physics. The work of the PI (AWL) and additional personnel is to provide theory input needed for a number of potentially high-impact experiments, notably, hadronic parity violation, Dark Matter direct detection and searches for permanent electric dipole moments (EDMs) in nucleons and nuclei. In all these examples, a quantitative understanding of low-energy nuclear physics from the fundamental theory of strong interactions, Quantum Chromo-Dynamics (QCD), is necessary to interpret the experimental results. The main theoretical tools used and developed in this work are the numerical solution to QCD known as lattice QCD (LQCD) and Effective Field Theory (EFT).

This grant is supporting a new research program for the PI, and as such, needed to be developed from the ground up. Therefore, the first fiscal year of this grant, 08/01/2014–07/31/2015, has been spent predominantly establishing this new research effort. Very good progress has been made, although, at this time, there are not many publications to show for the effort. The main goals of the research proposal in this fiscal year were to

1. perform an exploratory LQCD calculation at $m_\pi \sim 800$ MeV of the $\Delta I = 2$ hadronic parity violating matrix element in the two-nucleon system,

2. perform an exploratory LQCD calculation at $m_\pi \sim 400$ MeV of the scalar matrix elements in the nucleon, $m_q \langle N|\bar{q}q|N\rangle$ for quark flavors $q = \{s, c\}$, which are needed to interpret direct Dark Matter detection experiments,

3. compute the strong contribution to $m_n - m_p$ from $m_d - m_u$ and relate this to Big Bang Nucleosynthesis (BBN),

4. perform an exploratory calculation at $m_\pi \sim 800$ MeV of the CP-violating pion-nucleon coupling that would arise from a quark chromo-EDM operator from beyond the Standard Model Physics.

I summarize below the progress made towards these goals.

After one year, the PI accepted a job at Lawrence Berkeley National Laboratory, so this final report covers just a single year of five years of the grant.

1.2 Accomplishments

Significant progress has been made towards accomplishing several of the above research items.

Hadronic Parity Violation: Working with the SciDAC supported CalLat Collaboration, we developed a significantly improved basis of interpolating fields to compute properties of the two-nucleon system with LQCD. The improved methodology has allowed us to perform an exploratory calculation of the nucleon-nucleon S, P, D and F wave elastic scattering states. The key improvement over previous work was to construct sources for which the two-nucleons are physically displaced from one another. By varying the separation distance, the overlap of the source interpolating field on the various bound and scattering states varies, allowing us to easily identify the various states in the system very early in Euclidean time, such that a reliable extraction of the energy levels can be performed. We are preparing two publications on this work and expect them to be published this summer or fall.

The development of these interpolating fields is necessary to perform the LQCD calculation of hadronic parity violation. One can not simply compute the desired transition amplitudes as the finite volume matrix elements do not cleanly map one-to-one onto the infinite volume amplitudes of interest. The finite volume distorts the two-particle final state wave functions including a mixing of various partial waves since the LQCD calculations only respect 3-dimensional cubic symmetry. We have taken a first step towards computing the correction factor needed to map finite volume matrix elements to the infinite volume transition amplitude.[1] In Ref. [4], with R. Briceno and M. Hansen, I have determined the correction factor for a $1 \to 2$ transition form factor for scalar particles. We are currently working on the equivalent correction factor for $2 \to 2$ states with spin, relevant to electroweak matrix elements in the two nucleon system. We anticipate completing this formal development in the Fall.

With CalLat, we have begun the exploratory LQCD calculation of the $\Delta I = 2$ hadronic parity violating matrix element relevant to the experimental measurement of a parity violation in polarized $\vec{p}p$ scattering. The $\Delta I = 2$ matrix element is an ideal *laboratory* for investigating these types of LQCD calculations as the there are several simplifications that occur in the calculation of this observable, including the absence of quark disconnected diagrams and a lack of operator mixing, two of the most severe systematics to address in LQCD calculations. Further, to simplify the contractions, we are performing the calculation of the S to P wave, parity violating $nn \to pp$ matrix element. This greatly simplifies the Wick contractions and is simply related to the matrix element of interest through a Clebsch-Gordon coefficient. The determination of both the S and P wave scattering phase shifts (discussed above) are necessary to determine the finite volume correction factor to convert the finite volume LQCD calculations to the desired infinite volume transition amplitudes.

The numerical LQCD calculations are improved through an interface to the professionally maintained HDF5 High Performance Parallel I/O Library [10], which was developed with SciDAC support.

We realized the largest systematic uncertainty in our work remains the use of good two-nucleon interpolating fields. We have therefor paused this calculation to do more research and development on the two-nucleon elastic scattering interpolating operators.

Isospin violation and BBN: I hired a former graduate student from WM (Ekaterina Mastropas) in a temporary visiting position to help complete the LQCD calculation of the $m_d - m_u$ contribution to $M_n - M_p$. E. Mastropas was hired for 6 months, 3 paid by JLab and 3 from this grant. The work is nearly complete, however Dr. Mastropas had a second child in April, so the publication of the work has been delayed.

What was not appreciated before this work is that $m_n - m_p$ displays a very prominent chiral logarithm, see Fig. 1. This is a very significant result as the presence of chiral logarithms are predicted by chiral perturbation theory, and so the appearance of them in numerical LQCD results is a strong indicator that our understanding of low-energy chiral dynamics, based upon decades of phenomenology, is correct. In this work, we have found the first conclusive evidence of such a chiral logarithm in the baryon sector. This evidence is manifest in the strong curvature of $m_n - m_p$ as a function of the pion mass, Fig. 1. Such curvature from chiral logarithms can not be captured by low-orders in a taylor expansion, and are in some sense the most prominent predictions from low-energy effective field theories.

This project is being led by my two graduate students, David Brantley and Henry Monge Camacho. While this slowed down the progress, it was a great introductory project to get them

[1] These corrections are commonly know in the LQCD literature as Lellouch-Lüscher factors, named after the first two authors to determine such corrections, relevant for $K \to \pi\pi$ decays.

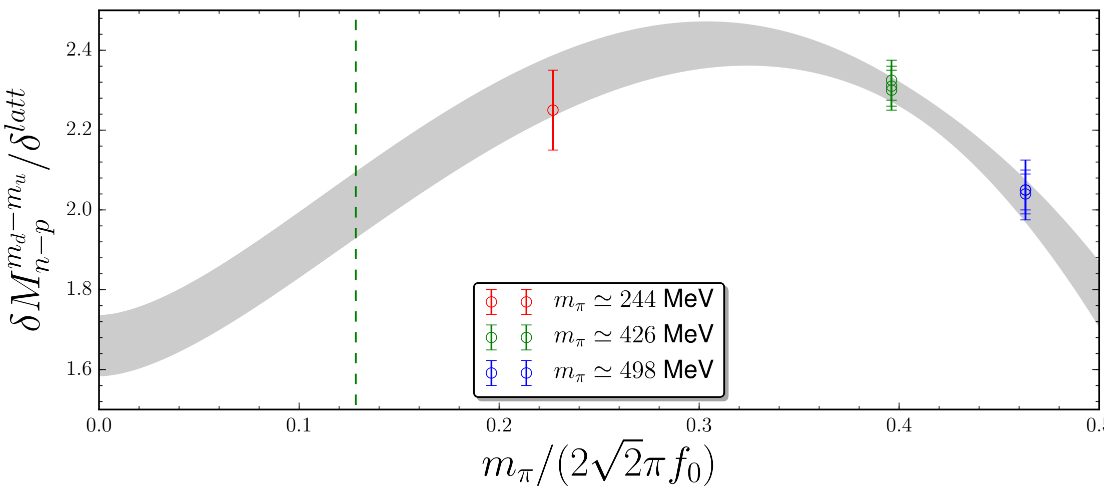

Figure 1: Preliminary LQCD determination of the isovector nucleon mass splitting from QCD, $\delta M_{n-p}^{m_d-m_u}$, scaled by the isovector quark mass $2\delta = m_d - m_u$ in lattice units, δ^{latt}. The strong curvature is driven by a chiral logarithm with a large coefficient. This is the first conclusive evidence for a chiral logarithm in the baryon sector when comparing lattice QCD to baryon chiral perturbation theory.

used to lattice QCD and effective field theory, preparing them for the main research efforts for the Ph.D. studies.

Quantifying Big Bang Nucleosynthesis sensitivity to isospin violation: Big Bang Nucleosynthesis (BBN) describes the production of light nuclear elements in the first few minutes after the big bang. With the basic nuclear reaction rates measured experimentally, and the primordial baryon to photon ratio determined from the Cosmic Microwave Background studies, BBN provides a parameter free prediction of the abundances of light nuclei in the early universe. As such, BBN is a common testing ground for constraining potential models of BSM physics. BBN is exquisitely sensitive to isospin breaking, as the isovector nucleon mass, $m_n - m_p$ sets the initial abundance of neutrons to protons and controls the lifetime of free neutrons. We now know quantitatively how the nucleon mass splitting arises from the two sources of isospin breaking: the down-up quark mass splitting and through the electromagnetic couplings of the quarks. This allows us to quantitatively explore variations of BBN predictions through simultaneous variation of both $m_d - m_u$ and $\alpha_{f.s.}$, and thus constrain BSM models through their predicted variations of these two isospin breaking parameters. This was a perfect project for an undergraduate physics major in their senior year, having been exposed to all the fundamental physics courses needed for modern physics: quantum mechanics, electromagnetism and statistical physics. It involved creating a simple python wrapper around the publicly available fortran bbn code that enabled control of all the quantities sensitive to isospin breaking. Matthew Heffernan was an enthusiastic undergraduate at W&M. I agreed to supervise him for his honors thesis project, which he successfully defended in May this year. The project was completed in collaboration with Projjwal Banerjee, a postdoc specializing in nuclear astrophysics. We are preparing a manuscript for publication based upon our work.

Massive QED: We have formulated and demonstrated a novel method of incorporating QED in LQCD calculations, **Massive QED** [2]. LQCD calculations have reached a level of maturity that isospin breaking from the $m_d - m_u$ quark mass operator and QED must be included to compare with experimental results. The standard method use the finite spatial volume to regulate the infrared (IR) photon effects, which lead to large power-law finite volume corrections that must be accounted for by performing the calculations in multiple lattice volumes (a numerically expensive endeavor). We proposed instead to use a photon mass term to regulate the IR physics. We were able to demonstrate that for equal computing time, one could achieve equal uncertainty by utilizing multiple photon masses on a single spatial volume. This method provides an alternate IR regulator to the standard method at less numerical cost and opens the door for computing charged particle interactions with LQCD + QED as the soft-photon radiation is regulated by the photon mass, providing a window to perform calculations of elastic scattering by turning off the Bremsstrahlung radiation.

CP violating matrix elements from the baryon spectrum: One of the main goals of the research supported by this grant is to determine CP-violating couplings arising from potential BSM sources of CP-violation. To achieve this goal, we aim to determine these couplings indirectly by examining the resulting modifications to the single baryon spectrum arising from these potential sources of BSM CP-violation and the related CP-conserving operators. To utilize this method, we must examine the relation and small corrections to them between the modification of the spectrum and the CP-violating matrix elements of interest. Working with Emanuele Mereghetti and Jordy de Vries, I have pushed the EFT calculations of this relation to next-to-next-to leading order (NNLO) in $SU(3)$ baryon chiral perturbation theory [3]. Critically, we were able to demonstrate that the classic relationship between $m_n - m_p$ and the CP-violating coupling g_0 arising from the QCD θ term is not spoiled by large $SU(3)$ flavor breaking corrections.

In addition to the accomplishments of the research, I have made the following progress in supporting the research plan outlined in the grant:

- A postdoctoral fellow has been successfully identified, Chia Cheng (Jason) Chang, to work with the PI. A job offer was made and accepted with an anticipated start date in the Fall of 2015.
- A research and development computing cluster was purchased, using $124,407 from the grant, with matching funds of $30,000 from the William & Mary (WM) physics department. The cluster has been installed and configured, and is being used by local personnel on research proposed in the original proposal.
- A former graduate student from WM (Ekaterina Mastropas) was hired in a temporary visiting scientist position for 6 months, 3 months paid by Jlab, and three from this grant, to conduct research related to the original proposal. We anticipate two publications from this work.
- Two WM graduate students (David Brantley and Henry Monge) will be paid this summer in part from funds from this grant to conduct research related to the original proposal.
- The research goals of this proposal have been widely disseminated by the PI in numerous conference presentations, seminars, colloquium and summer school lectures.

Publications: Publications:

[1] *Two-Nucleon Higher Partial-Wave Scattering from Lattice QCD*,
E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P. Vranas and A. Walker-Loud, *in the referee process*,
`http://arXiv.org/abs/arXiv:1508.00886`.

[2] *Massive photons: an infrared regularization scheme for lattice QCD+QED*,
M. G. Endres, A. Shindler, B. C. Tiburzi and A. Walker-Loud,
accepted for publication in **Phys. Rev. Lett**, (2016),
http://arXiv.org/abs/arXiv:1507.08916.

[3] *Baryon mass splittings and strong CP violation in* $SU(3)$ *Chiral Perturbation Theory*,
J. de Vries, E. Mereghetti and A. Walker-Loud, **Phys. Rev. C 92**, 045201 (2015),
http://arXiv.org/abs/arXiv:1506.06247.

[4] *Multichannel* $1 \to 2$ *transition amplitudes in a finite volume*,
R. A. Briceo, M. T. Hansen and A. Walker-Loud, **Phys. Rev. D 91**, 034501 (2015),
http://arXiv.org/abs/arXiv:1406.5965.

[5] *High-Performance I/O: HDF5 for Lattice QCD*,
T. Kurth, A. Pochinsky, A. Sarje, S. Syritsyn and A. Walker-Loud, **PoS** LATTICE **2014**, 045, http://arXiv.org/abs/arXiv:1501.06992.

Conference Proceedings:

[6] *Photon mass term as an IR regularization for QCD+QED on the lattice*,
M. G. Endres, A. Shindler, B. C. Tiburzi and A. Walker-Loud, **PoS** LATTICE **2015**,
http://arXiv.org/abs/arXiv:1512.08983.

[7] *Two-nucleon scattering in multiple partial waves*,
E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P. Vranas and A. Walker-Loud, **PoS** LATTICE **2015**,
http://arXiv.org/abs/arXiv:1511.02262.

[8] *Nuclear Parity Violation from Lattice QCD*,
E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P. Vranas and A. Walker-Loud, **PoS** LATTICE **2015**,
http://arXiv.org/abs/arXiv:1511.02260.

[9] *Multichannel one-to-two transition amplitudes in a finite volume*,
R. A. Briceo, M. T. Hansen and A. Walker-Loud, **PoS** LATTICE **2014**, 095,
http://arXiv.org/abs/arXiv:1502.00540.

[10] *High-Performance I/O: HDF5 for Lattice QCD*,
T. Kurth, A. Pochinsky, A. Sarje, S. Syritsyn and A. Walker-Loud, **PoS** LATTICE **2014**, 045, http://arXiv.org/abs/arXiv:1501.06992.

Invited Conference/Workshop Talks:

[11] *Isospin Violation and QCD*, Workshop on Bound States and Resonances in EFT and Lattice QCD, Benasque, Spain, August 2014.

[12] *CP-Violating pion-nucleon couplings from quark chromo-EDMs*, Proton Structure Meeting, 18-19 September, 2014, SURA Conference Center, DC.

[13] *Status of scalar quark matrix elements from Lattice QCD*, INT Workshop on Dark Matter, December, 2014.

[14] *CP-Violating pion-nucleon couplings from quark chromo-EDMs*, Amherst Center for Fundamental Interactions workshop on Hadronic Matrix Elements for Probes of CP-Violation, January, 2015.

[15] *Precision tests of the Standard Model and low-energy nuclear physics*, colloquium at San Francisco State University, February 2015.

[16] $M_n - M_p$, seminar at the Amherst Center for Fundamental Interactions, February, 2015.

[17] *Nucleon-Nucleon interactions and nuclear structure on the lattice*, plenary talk at the Quarks and Nuclear Physics Conference in Valparaíso, Chile, March, 2015.

[18] $M_n - M_p$, seminar for the High Energy Theory Group at Michigan State University, April 2015.

[19] *Precision low-energy nuclear physics in the age of High Performance Computing*, colloquium at the University of Arizona, April 2015.

[20] $M_n - M_p$, Heavy Ion Tea Seminar for the Nuclear Science Division at Lawrence Berkeley National Laboratory, May 2015.

Invited Lectures:

[21] *Introduction to Lattice QCD and calculations of nucleon matrix elements*, lectures for the 17th Taiwan Nuclear Physics Summer School held at the Institute of Physics, Academica Sinica, Taiwan, August 2014.

[22] *Connecting Nuclear Physics to QCD with the lattice*, lectures for the Helmholtz International Summer School held at the Bogoliubov Laboratory of Theoretical Physics at the Joint Institute for Nuclear Research in Dubna, Russia, August/September 2014.

2 Participants

Other Senior Staff: There are a few other key senior personnel collaborating on the research related to or supported by this award, supported through their own institutions and grants.

- **Kate Clark** is a software developer at NVIDIA Corporation. Kate has a background in lattice field theory and is the world expert on writing performant libraries for NVIDIA GPU architectures, contained in the library `QUDA`, of which she is the principle developer. The research we perform greatly benefits from the continued development of `QUDA`. Our calculations receive an $\mathcal{O}(100)$ speed up using NVIDIA GPUs as compared to traditional CPU architectures.

- **Wick Haxton** is a Senior Staff Scientist at LBNL and Professor of Physics at UC Berkeley. Wick is developing HOBET (Harmonic Oscillator Based Effective Theory), a low-energy description of two and more nucleon interactions. We are coordinating with Wick and collaborators to match some of our lattice QCD results to HOBET so we can extend the application of our research to nuclei.

- **Balint Joo** is a Senior Staff Scientist at Thomas Jefferson National Laboratory. Balint is the preeminent expert on developing lattice QCD software for applications to low-energy nuclear physics. Balint has been instrumental in adding required features to the `Chroma` software suite that have enabled the research supported by this grant. He continues to work closely with us in developing software and assisting in compiling our code on various supercomputing centers.

- **Thorsten Kurth** was a postdoc at LBNL and is now a Staff Scientist at NERSC. Thorsten has been the main software developer for lattice QCD code used by our collaboration, `latscat`. While Thorsten is now preoccupied with his new job, he remains engaged in our research endeavors and still helps develop our software, though primarily now by consulting. We are applying to various other funding opportunities to find funds to pay Thorsten part time to work more closely with us.

- **Kostas Orginos** is a Professor at The College of William & Mary and Senior Staff Scientist at Thomas Jefferson National Laboratory. Kostas is a world expert in applying lattice QCD to low-energy nuclear physics problems. I have a longstanding collaborative relationship with Kostas and we continue to work together.

- **Pavlos Vranas** is a Senior Staff Scientist at Lawrence Livermore National Laboratory. He is a leading expert on lattice field theory with an emphasis towards particle physics, and the original architect of the widely used `CPS` lattice field theory software. Pavlos Vranas and I are the lead lattice experts in the CalLat collaboration, aimed at applying lattice QCD to low-energy nuclear physics. Pavlos is additionally instrumental in acquiring computing allocations on the LLNL supercomputers.

Postdocs: There are a number of postdocs collaborating with me on research supported in this grant. This year, we successfully hired Chia Cheng (Jason) Chang, who is supported fully by this grant. The other postdocs are funded through other grants but collaborate on research supporting this grant.

- **Projjwal Banerjee** is a postdoctoral research associate at the University of Minnesota. Projwall is an expert in nuclear astrophysics and has been collaborating on interfacing lattice QCD results and Big Bang Nucleosynthesis.

- **Chris Bouchard** is currently a postdoctoral fellow at W&M, supported by the DOE grant of K. Orginos. He has accepted a faculty position at the University of Glasgow which he will be starting this fall. Chris has been instrumental in developing our new Feynman-Hellman approach to hadronic matrix elements.

- **Evan Berkowitz** is a postdoctoral research associate at LLNL and will be moving to Julich to work with Tom Luu (a regular collaborator of mine in the past). Evan expects to stay actively involved in research efforts aligned with this grant, and we hope to find projects with which to also collaborate with Tom Luu regarding lattice QCD applied to few-baryon systems. Evan has become one of the main software developers of `latscat` with guidance from Thorsten Kurth, being the one to code our newest two-nucleon operators, in addition to contributing to the development of new ideas.

- **Chia Cheng (Jason) Chang** is a postdoctoral fellow at LBNL supported by this grant. Jason has been an outstanding hire and has been instrumental in setting up our new database to foster improved sharing of lattice results within our collaboration. He is also helping to develop new and improved ideas for computing hadronic matrix elements and is actively involved in the lattice QCD calculations supporting this research grant. I could not be happier with his progress, Jason is an exceptional young physicist.

- **Emanuele Mereghetti** is a postdoctoral fellow at LANL. Emanuele is an expert in effective field theory for CP-violation in low-energy nuclear physics (among other things). Emanuele and I began collaborating when we were both postdocs at LBNL. Conversations with Emanuele developed into a significant aspect of the research supported by this grant. We continue to collaborate together on various EFT calculations relevant to CP-violation and Emanuele continues to be involved in the relevant LQCD calculations.

- **Amy Nicholson** is a postdoctoral research fellow at UC Berkeley, supported by Wick Haxton's DOE research grant. Amy is an expert in low-energy multi-nucleon systems and also lattice QCD applied to low-energy nuclear physics. Amy has contributed significantly to research supported by this grant, notably helping to design our newest two-nucleon operators.

- **Enrico Rinaldi** is a postdoctoral research associate at LLNL and an expert of applying lattice field theory to BSM models. Enrico has accepted a RIKEN Fellowship to work at BNL as an independent scientist and expects to remain involved in research supported by this grant. Enrico has been instrumental in getting this research program to work on the various computing facilities we have access to, including the various machines at LLNL as well as on Titan at OLCF.

Students: During the first fiscal year, there have been three graduate students involved in the research and one undergraduate student has begun research.

- **Michael Freid** has completed his fourth year of graduate school at W&M. Michael is working closely with Carl Carlson. We plan to investigate a new renormalization technique developed by Kostas and Chris Monahan to apply to the lattice QCD calculations of the operators related to CP-violation.

- **David Brantley** just completed his thrid year of graduate school at W&M. He received a DOE SCGSR Award for 12 months to work with me at LBNL on the research supported in this grant. David is additionally supported in part by a DOE Topical Collaboration Grant I received (while still at W&M) on neutrinoless double beta-decay and fundamental symmetry tests. The SCGSR Award supports David's salary for 12 months (June 1, 2016 – May 31, 2017), after which he will be supported in part by the Topical Collaboration grant and this grant. Additional funding will be needed to support David through completing his Ph.D. studies, which will be focussed on the CP-violating aspect of the research supported by this grant.

- **Ken McElvain** is currently a graduate student at UC Berkeley working under the supervision of W. Haxton. His research topic is the direct derivation of nuclear effective theory from energy levels and boundary conditions, which can be used in this project to make the connection from LQCD to nuclear physics. Ken has extensive(20+ years) industry experience with technical software development. He has also contributed extensively to the parallelization of BIGSTICK, a leading nuclear shell model code, using both MPI and OpenMP. Ken developed the initial implementation of `mpi_jm`, a C++ based MPI job manager which we expect to lower the overhead for scheduling tasks as well as enable running CPU and GPU intensive jobs on the same nodes.

- **Henry Monge Camacho** just completed his second year of graduate school at W&M. Henry is supported primarily through the above mentioned DOE Topical Collaboration Grant, with supplemental support coming from this grant. With this support, Henry was also able to

Table 1: Graduate and Undergraduate Students

Student	Entered Grad School	Joined Group	Degree	Date Degree Expected	Advisor	Support
Michael Fried	8/12 WM	1/15	Ph.D.	5/17	Walker-Loud	JLab
David Brantley	8/13 WM	3/15	Ph.D.	5/18	Walker-Loud	Grant/TA
Henry Monge	8/14 WM	3/15	Ph.D.	5/19	Walker-Loud	Grant/TA
Matt Heffernan	–	4/15	Bs.Sc.	5/16	Walker-Loud	unsupported

Table 2: Project Participants. I list all the young scientists participating in the work who are working to find a permanent academic/research position.

Name	Capacity	Dates	Research Area	Support
Projjwal Banerjee	Postdoc	8/15 –present	Astrophysics	Minnesota
Evan Berkowitz	Postdoc	8/14 –present	LQCD	LLNL
Chris Bouchard	Postdoc (Professor)	8/14 –present	LQCD	Orginos Grant
Chia Cheng (Jason) Chang	Postdoc	9/15–8/18	LQCD	ECA
Emanuele Mereghetti	Postdoc	8/14–present	EFT/LQCD	LANL
Amy Nicholson	Postdoc	8/15–present	EFT/LQCD	Haxton Grant
Enrico Rinaldi	Postdoc	8/14 –present	LQCD	LLNL
André Walker-Loud	Staff	8/13 – present	LQCD and EFT	LBNL

move to the Bay Area to work closely with me while finishing his Ph.D. studies. Henry's research will be focussed on using lattice QCD to assist in theoretical support for neutrinoless double beta-decay searches. This work requires development of improved two-nucleon lattice QCD calculations, and also will parallel the hadronic parity violating calculations we are performing. The similarity of the calculations will allow Henry to contribute to both meaningfully. Additional funding will be required to support Henry through the completion of his Ph.D. studies.

- **Matt Heffernan** just graduated from W&M with honors and will be attending McGill University of graduate school. Matt was a very motivated young student and for his undergraduate research thesis, along with Projwall Banerjee, interfaced lattice QCD results on isospin breaking and Big Bang Nucleosynthesis. We are currently writing a scientific publication based upon his work.