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Properties of Nuclei up to $A = 16$ using Local Chiral Interactions

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We report accurate quantum Monte Carlo calculations of nuclei up to $A = 16$ based on local chiral two- and three-nucleon interactions up to next-to-next-to-leading order. We examine the theoretical uncertainties associated with the chiral expansion and the cutoff in the theory, as well as the associated operator choices in the three-nucleon interactions. While in light nuclei the cutoff variation and systematic uncertainties are rather small, in ^{16}O these can be significant for large coordinate-space cutoffs. Overall, we show that chiral interactions constructed to reproduce properties of very light systems and nucleon-nucleon scattering give an excellent description of binding energies, charge radii, and form factors for all these nuclei, including open-shell systems in $A = 6$ and 12.

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Introduction.—Predicting the emergence of nuclear properties and structure from first principles is a formidable task. An important open question is whether it is possible to describe nuclei and their global properties, e.g., binding energies and radii, from microscopic nuclear Hamiltonians constructed to reproduce only few-body observables, while simultaneously predicting properties of matter, including the equation of state and the properties of neutron stars. Despite advanced efforts, definitive answers are not yet available [1–9].

Several properties of nuclei up to ^{12}C have been successfully described using the phenomenological Argonne v_{18} (AV18) nucleon-nucleon (NN) potential combined with Illinois models for the three-body interactions [5]. Unfortunately these phenomenological models have at least two main limitations. They do not provide a systematic way to improve the interactions or to estimate theoretical uncertainties. In addition, they provide a too soft equation of state of neutron matter [10, 11], with the consequence that the predicted structure of neutron stars is not compatible with recent observations of two solar-mass stars [12, 13].

The Argonne-Illinois models have been constructed to be nearly local: The dominant parts of the interaction do not depend on the momenta of the two interacting nucleons but only on their relative distance, spin, and isospin. This construction was motivated by the ease of employing such potentials in continuum quantum Monte Carlo (QMC) methods, such as the Green's function Monte Carlo (GFMC) and auxiliary field diffusion Monte Carlo (AFDMC) methods. The advantage of QMC methods is that they can be used to solve accurately and nonperturbatively the many-body problem without requiring the use of softer Hamiltonians. The GFMC and AFDMC methods can be successfully used only for nearly local Hamiltonians because of the sign problem [5].

In the last two decades, chiral effective field theory (EFT) has paved the way to the development of nuclear interactions and currents in a systematic way [14, 15]. Chiral EFT expands the nuclear interaction in the ratio of a small scale (e.g., the pion mass or a typical momentum scale in the nucleus) to a hard scale (the chiral breakdown scale). Such an expansion provides several advantages over the traditional approach, including the ability to improve the interaction order by order, means to estimate theoretical uncertainties, and the fact that many-body forces and currents are predicted consistently. The long-range pion-exchange contributions are determined by pion-nucleon couplings, while the short-range contributions (given by so-called low-energy constants) are fit to reproduce experimental data. Usually, chiral EFT interactions are formulated in momentum space, but recently Gezerlis *et al.* demonstrated a way to produce equivalent local formulations of chiral NN interactions up to next-to-next-to-leading-order (N^{2}LO) [16, 17]. Consistent three-body forces were constructed in Refs. [18–20], as well as chiral interactions with explicit Delta degrees of freedom [21–24].

To solve for the ground state of nuclei, we use the AFDMC method with local chiral interactions that have been determined from fits to NN scattering, the alpha particle binding energy, and n–α scattering [19, 20]. This method has previously been used to determine the properties of homogeneous and inhomogeneous neutron matter [25–28], and nuclear matter and finite nuclei using simplified potentials [29].

In this Letter we present several new important achievements: (i) the first application of the AFDMC method to calculate properties of nuclei using chiral Hamiltonians at N^{2}LO, including three-body forces, (ii) a systematic investigation of the chiral expansion, including truncation error estimates, in selected nuclei from

$A = 3$ to $A = 16$, and (iii) an investigation of the cutoff dependence and the use of different three-body operators for $A \geq 6$.

Hamiltonian and AFDMC method.—The Hamiltonian is of the form

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}\,, \qquad (1)$$

where the two-body interaction v_{ij} also includes Coulomb and other electromagnetic effects. The two-body potentials v_{ij} and three-body potential V_{ijk} are as in Refs. [16–20]. The general form of the variational state is the following:

$$|\Psi\rangle = [F_C + F_2 + F_3]|\Phi\rangle_{J,T}\,, \qquad (2)$$

where F_C accounts for all the spin- and isospin-independent correlations, and F_2 and F_3 are linear in spin- and isospin-pair two- and three-body correlations as described in Ref. [5].

The term $|\Phi\rangle$ is taken to be a shell-model-like state with total angular momentum J and total isospin T. Its wave function consists of a sum of Slater determinants D constructed using single-particle orbitals:

$$\langle RS|\Phi\rangle_{J,T} = \sum_n c_n \left(\sum D\{\phi_\alpha(\mathbf{r}_i, s_i)\}\right)_{J,T}\,, \qquad (3)$$

where $\mathbf{r}_i$ are the spatial coordinates of the nucleons and s_i represent their spins. Each single particle orbital ϕ_α consists of a radial function $\varphi(r)$ coupled to the spin and isospin states. The determinants are coupled with Clebsch-Gordan coefficients to total J and T, and the c_n are variational parameters multiplying different components having the same quantum numbers. The radial functions $\varphi(r)$ are obtained by solving for the eigenfunctions of a Wood-Saxon well, and all parameters are chosen by minimizing the variational energy as described in Ref. [30]. In order to improve $|\Phi\rangle$, we include single particle orbitals up to the *sd* shell.

A complete description of the AFDMC method using two-body interactions is given in Refs. [5, 31]. Here we describe how three-body interactions are included. The main limitation of the AFDMC method is that the standard Hubbard-Stratonovich transformation used to propagate the wave function in imaginary time can only be applied to potentials that are quadratic in spin and isospin operators. The three-body coordinate-space dependence is straightforward to include, as are several important terms in the three-body interaction that depend on the spin and isospin of two nucleons at a time. Terms depending on the spin and isospin of all three nucleons are included in an effective way in the propagation, and then fully accounted for in the final results. In practice, we determine a Hamiltonian H' that mimics the full Hamiltonian, as discussed in the following, and then we calculate as a perturbation the difference $\langle H' - H\rangle$. This procedure goes beyond the standard normal ordering that averages the dependence of the third nucleon's position, spin, and isospin.

The chiral three-body interactions at N^{2}LO contain terms that can be organized as

$$V = V_a^{2\pi,P} + V_c^{2\pi,P} + V^{2\pi,S} + V_D + V_E\,. \qquad (4)$$

The first, second, and third terms correspond to the two-pion exchange diagrams in P and S waves [Eqs. (A.1b), (A.1c) and (A.1a), respectively, of Ref. [20]]. The subscripts a and c refer to the fact that these contributions can be written in terms of an anticommutator or commutator, respectively. We can rewrite $V_{a,c}^{2\pi,P}$ by separating it into long-, intermediate-, and short-range parts:

$$V_{a,c}^{2\pi,P} = V_{a,c}^{XX} + V_{a,c}^{X\delta} + V_{a,c}^{\delta\delta}\,, \qquad (5)$$

where X and δ refer to the $X_{ij}(\mathbf{r})$ and $\delta_{R_{3N}}(\mathbf{r})$ functions defined in Ref. [20]. V_D contains an intermediate-range one-pion-exchange-contact interaction [Eq. (24b) of Ref. [20]], while V_E contains a short-range term. In this work, we consider two alternative forms for V_E: namely, $V_{E\tau}$ and $V_{E\mathbb{1}}$ [Eqs. (26a) and (26b), respectively, of Ref. [20]]. They differ in the operator structure, according to the Fierz-rearrangement freedom in the selection of local contact operators in the three-body sector up to N^{2}LO [32]. $E\tau$ refers to the choice of the two-body operator $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, while $E\mathbb{1}$ to the choice of the identity operator $\mathbb{1}$.

The terms $V_a^{2\pi,P}$, $V^{2\pi,S}$, V_D, and V_E are purely quadratic in spin and isospin operators, and can be included exactly in the AFDMC propagator. The term $V_c^{2\pi,P}$ contains instead explicit cubic spin and isospin operators. These terms cannot be fully included in the AFDMC propagation; however, their expectation value can be calculated. We determine the Hamiltonian H' that can be fully propagated as

$$H' = H - V_c^{2\pi,P} + \alpha_1 V_a^{XX} + \alpha_2 V_D + \alpha_3 V_E\,. \qquad (6)$$

The three constants α_i are adjusted in order to have

$$\begin{aligned} \langle V_c^{XX}\rangle &\approx \langle \alpha_1 V_a^{XX}\rangle\,, \\ \langle V_c^{X\delta}\rangle &\approx \langle \alpha_2 V_D\rangle\,, \\ \langle V_c^{\delta\delta}\rangle &\approx \langle \alpha_3 V_E\rangle\,, \end{aligned} \qquad (7)$$

where the identifications are suggested by the similar ranges and functional forms. The average $\langle\cdots\rangle$ indicates an average over the propagated wave function. Once the ground state Ψ of H' is calculated with the AFDMC method, the expectation value of the Hamiltonian H is given by

$$\langle H\rangle \approx \langle\Psi|H'|\Psi\rangle - \langle\Psi|H' - H|\Psi\rangle\,, \qquad (8)$$

where the last quantity in the previous expression is evaluated perturbatively. Adjusting the constants α_i in such a way that the correction is small suggests that the correction is perturbative. The same estimate is used in GFMC calculations to determine the small contributions from nonlocal terms that are present in the AV18 potential, and in that case the difference $v_8' - v_{18}$ is calculated as a perturbation [33].

In order to test the technique described above, we first determined the optimal parameters α_i for a given system, then changed their values by up to 10%, and verified that the final result of $\langle H \rangle$ is nearly independent of such a variation. For example, for ^{16}O such a variation changes $\langle H' - H \rangle$ from ≈ 1 to ≈ 15 MeV, but the final estimate of the ground-state energy is within 2 MeV. In addition, we benchmarked the energies of $A = 3$ and $A = 4$ nuclei using the AFDMC method, by comparing with the GFMC results of Refs. [19, 20], where the three-body interactions are included fully in the propagation and found very good agreement within a few percent. Note that in many other approaches the three-body force is replaced by an effective two-body interaction (this is achieved by normal ordering) neglecting the residual three-body term [34, 35]. However, this approximation has only been benchmarked for softer interactions [36, 37].

The AFDMC method used here is limited by a sign problem [29, 31]. The sign problem is initially suppressed by evolving the wave function in imaginary time using the constrained-path approximation, where the configurations are constrained to have positive real overlap with the trial function, as described in Ref. [38]. After an initial equilibration of the configurations using the constrained-path approximation, the constraint is removed, and then the evolution in imaginary-time is performed until the sign-problem dominates and the variance of the results becomes severely large. The final (statistical) error strongly depends on the quality of the trial wave function. We have made several tests to check the results and the dependence on the initial trial wave function, and have concluded that the systematic uncertainties due to releasing the constraint give results correct to $\sim 5\%$ for ^{16}O. Initial attempts to improve the wave function for ^{16}O show a lowering of the energy by about $4 - 5$ MeV, but since the computational cost is much higher and statistical errors are similar to this difference, we leave more detailed studies to future work.

Results.—We consider chiral Hamiltonians at leading-order (LO), next-to-leading order (NLO), and N^{2}LO. In this way, following Ref. [39], we can assign theoretical uncertainties to observables coming from the truncation of the chiral expansion. Uncertainties for an observable X are estimated as $\Delta X^{\mathrm{N^2LO}} = \max(Q^4 \times |X^{\mathrm{LO}}|, Q^2 \times |X^{\mathrm{NLO}} - X^{\mathrm{LO}}|, Q \times |X^{\mathrm{N^2LO}} - X^{\mathrm{NLO}}|)$, where we take $Q = m_\pi/\Lambda_b$ with $\Lambda_b = 600$ MeV (see Ref. [20] for a detailed discussion on uncertainty estimates with local chiral interactions).

Table I. Ground-state energies and charge radii for $A = 6$, 12, and 16 obtained for the N^{2}LO interactions with different cutoffs R_0 and different three-body interactions. The first uncertainty listed is statistical while the second is systematic. Experimental results are also shown.

Nucleus	V_E, R_0 (fm)	E_{AFDMC} (MeV)	r_{ch} (fm)
^{6}He	$E\tau$, 1.0	$-28.4(4)(2.0)$	1.99(4)(8)
	$E\mathbb{1}$, 1.0	$-28.2(5)(1.9)$	2.01(4)(7)
	$E\tau$, 1.2	$-29.3(1)(1.8)$	1.92(4)(8)
	Exp	-29.3	2.068(11) [42]
^{6}Li	$E\tau$, 1.0	$-31.5(5)(2.3)$	2.33(4)(10)
	$E\mathbb{1}$, 1.0	$-30.7(4)(2.1)$	2.33(4)(10)
	$E\tau$, 1.2	$-32.3(3)(1.7)$	2.24(4)(6)
	Exp	-32.0	2.589(39) [43]
^{12}C	$E\tau$, 1.0	$-78(3)(9)$	2.48(4)(18)
	Exp	-92.2	2.471(6) [44]
^{16}O	$E\tau$, 1.0	$-117(5)(16)$	2.71(5)(13)
	$E\mathbb{1}$, 1.0	$-115(6)(15)$	2.72(5)(11)
	$E\tau$, 1.2	$-263(26)(56)$	2.17(5)(11)
	Exp	-127.6	2.730(25) [45]

In Table I we report the AFDMC results for the ground-state energies and charge radii for nuclei with $A \geq 6$ at N^{2}LO. In particular, we used the two different cutoffs $R_0 = 1.0$ and $R_0 = 1.2$ fm (approximately corresponding to cutoffs in momentum space of 500 and 400 MeV [20], note, however also Ref. [40]), and two of the three available V_E interactions constructed in Ref. [19]. We find that, starting from local chiral Hamiltonians fit to NN scattering data [17] and three-body interactions fit to light nuclei [19, 20], energies and radii for nuclei up to $A = 16$ are qualitatively well reproduced. In particular, we find that the two cutoffs employed here, $R_0 = 1.0$ and $R_0 = 1.2$ fm, reproduce experimental binding energies and charge radii up to $A = 6$ within a few percent. An exception is for the charge radius of ^{6}Li that is slightly underestimated for both cutoffs. Sizably different is the case of the softer interaction ($R_0 = 1.2$ fm) for larger systems, which can significantly overbind ^{16}O, resulting in a very compact system. In this case the theoretical uncertainties on the energy are large, dominated by the severe overbinding at LO (≈ -1110 MeV).

We also find that the two different forms ($E\tau$, $E\mathbb{1}$) for the three-body interaction give similar results (agreeing within the EFT uncertainty) for nuclei up to $A = 16$. This suggests that the theoretical uncertainties coming from the truncation of the chiral expansion are sufficient to account for the violation of the Fierz rearrangement [19, 41].

In Fig. 1 we present the ground-state energies per nucleon of selected nuclei with $3 \leq A \leq 16$, calculated at LO, NLO, and N^{2}LO ($E\tau$) with the cutoff $R_0 = 1.0$ fm.

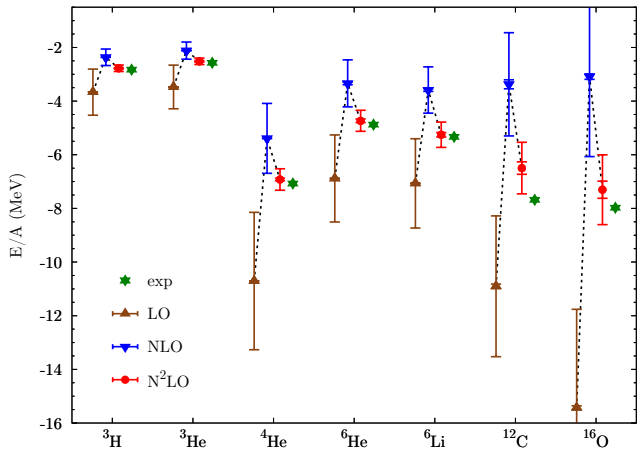

Figure 1. Ground-state energies per nucleon for $3 \leq A \leq 16$ up to N^{2}LO ($E\tau$) with the $R_0 = 1.0$ fm cutoff. Smaller error bars (indistinguishable from the symbols up to $A = 6$) indicate the statistical Monte Carlo uncertainty, while larger error bars are the uncertainties from the truncation of the chiral expansion.

The error bars are estimated by including the statistical uncertainties given by the AFDMC calculations as well as the error given by the truncation of the chiral expansion. The ground-state energies per nucleon are in agreement with experimental data up to $A = 6$, while for ^{12}C and ^{16}O the energies are somewhat underpredicted. The uncertainties are reasonably small, dominated by the truncation error.

In Fig. 2 we compare the charge radii calculated at LO, NLO, and N^{2}LO ($E\tau$) with the $R_0 = 1.0$ fm cutoff to experimental data. These results show that a qualitative description of binding energies and charge radii is possible starting from Hamiltonians constructed using only few-body data. We note, however, that the radius of ^{6}Li is slightly smaller than the experimental measurement. It is interesting to note that the charge radius of ^{6}Li calculated with the GFMC method employing the AV18 and Illinois VII (IL7) three-body interactions is also underestimated [5].

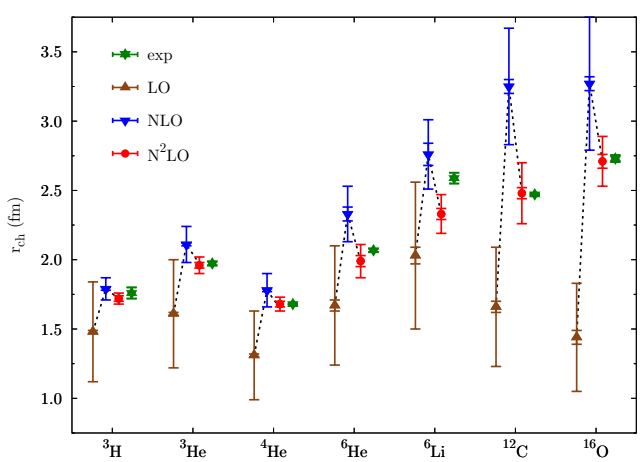

Figure 2. Charge radii for $3 \leq A \leq 16$ up to N^{2}LO ($E\tau$) with the $R_0 = 1.0$ fm cutoff. Error bars are as in Fig. 1.

We show in Fig. 3 the charge form factors of ^{12}C and ^{16}O compared to experimental data. The ^{12}C form factor is also compared to previous GFMC calculations with the AV18+IL7 potentials. Our form factor calculations have been performed using one-body charge operators only. Two-body operators are expected to give small contributions only at momenta larger than ≈ 500 MeV [46, 47], as they basically include relativistic corrections. It is interesting to compare the curves given by the two different cutoffs. In the figure, the result obtained using $R_0 = 1.0$ fm at N^{2}LO ($E\tau$) (solid blue line) includes the uncertainty from the truncation of the chiral expansion (shaded blue area). The agreement with experimental data is very good. For $R_0 = 1.2$ fm at N^{2}LO ($E\tau$) (dotted red line), the radius is too small and the first diffraction minimum occurs at a significantly higher momentum than experimentally observed, consistent with the overbinding obtained for this interaction.

Finally, in Fig. 4 we present the Coulomb sum rules for ^{12}C and ^{16}O. The AFDMC result for ^{12}C is compatible both with the available experimental data as extracted in

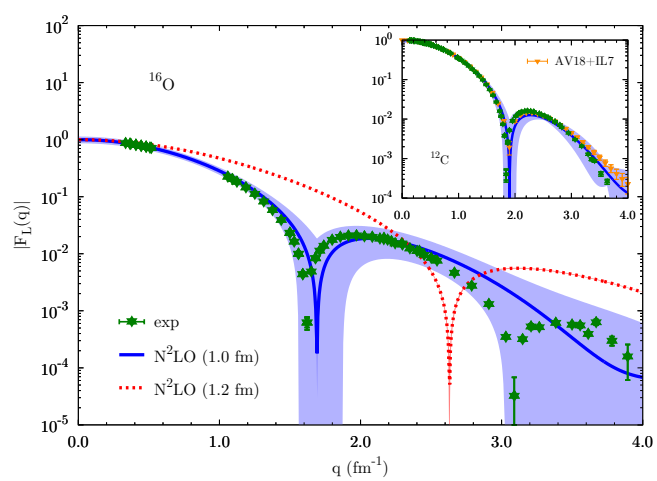

Figure 3. Charge form factor for ^{16}O at N^{2}LO for $R_0 = 1.0$ and 1.2 fm compared to experimental data [45, 48, 49]. For $R_0 = 1.0$ fm, both $E\tau$ and $E\mathbb{1}$ three-body operators give consistent results. The shaded area indicates the statistical Monte Carlo uncertainty combined with the (dominant) uncertainty from the truncation of the chiral expansion. For ^{12}C, AFDMC results are shown in the inset for $R_0 = 1.0$ fm versus experimental data from Ref. [50] and the GFMC results employing the AV18+IL7 potentials [46].

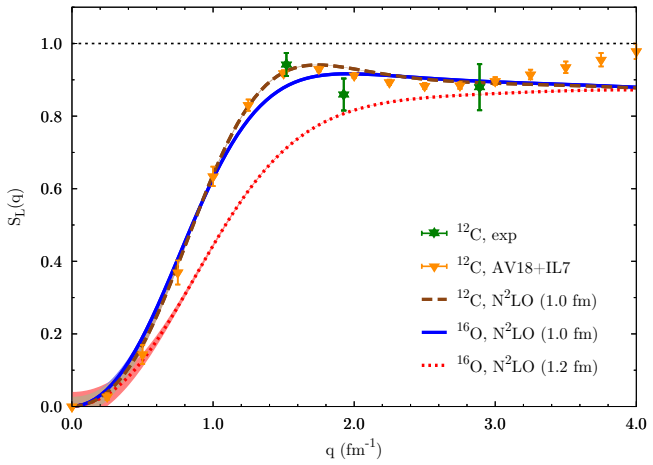

Figure 4. Coulomb sum rules for ^{12}C and ^{16}O at N^{2}LO ($E\tau$) compared to experimental data as derived in Ref. [51]. Results are shown for $R_0 = 1.0$ and 1.2 fm for ^{16}O, and for $R_0 = 1.0$ fm for ^{12}C. Shaded areas indicate only the statistical Monte Carlo uncertainty. In addition, we compare our results to GFMC calculations for ^{12}C with AV18+IL7 [46].

Ref. [51] and with the GFMC result for AV18+IL7 [46]. The differences between the AFDMC and GFMC results at high momentum are due to two-body currents, fully implemented to date only in the GFMC calculations. For ^{16}O, the result for the harder interaction with $R_0 = 1.0$ fm is very close to that of ^{12}C, and is compatible with the findings of Ref. [52] for the AV18+UIX potential. The softer interaction with $R_0 = 1.2$ fm produces instead a significantly different result, as for the charge form factor.

Summary.—We have performed QMC calculations of selected nuclei up to $A = 16$ using local chiral interactions at LO, NLO, and N^{2}LO for different cutoffs and three-body interactions. We conclude that these Hamiltonians, constructed only from NN data and properties of few-body nuclei, can give a good description of ground-state properties of nuclei up to $A = 16$, including binding energies, charge radii, form factors, and Coulomb sum rules. This is true in particular for the harder interaction considered here, corresponding to coordinate-space cutoff $R_0 = 1.0$ fm. For the larger cutoff $R_0 = 1.2$ fm, we find in ^{16}O a strong dependence of the energy uncertainty coming from the truncation of the chiral expansion, and a large overbinding and compactness. The latter two could be a consequence of the large c_D coupling in the $E\tau$ parametrization of the three-body force [19], resulting in a sizable attractive contribution not present in the hard interaction ($c_D = 0$). More detailed analysis to further investigate this behavior will be performed in future works.

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