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From the lightest nuclei to the equation of state of asymmetric nuclear matter with realistic nuclear interactions

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We present microscopic calculations of light and medium mass nuclei and the equation of state of symmetric and asymmetric nuclear matter using different nucleon-nucleon interactions, including a new Argonne version that has the same spin-isospin structure as local chiral forces at next-to-next-to-leading order. The calculations are performed using auxiliary field diffusion Monte Carlo (AFDMC) combined with an improved variational wave function and sampling technique. The AFDMC method can now be used to successfully calculate the energies of very light to medium mass nuclei as well as the energy of isospin-asymmetric nuclear matter, demonstrating microscopically the quadratic dependence of the energy on the symmetry energy.

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A fundamental challenge in nuclear physics is to calculate the properties of nuclei and nucleonic matter from realistic two- and three-nucleon interactions that reproduce measured phase shifts. Calculations based on these realistic interactions will be able to predict accurately properties of nuclei at higher-momentum transfer and of exotic states, including neutron star matter at higher densities.

The knowledge of the equation of state (EOS) of nuclear matter, particularly with different proton fractions (arbitrary isospin asymmetry), is of fundamental importance for both nuclear physics and astrophysics. The study of asymmetric matter enables further constraints on the bulk properties of nuclear density functionals often used to predict the properties of heavy nuclei including those with large neutron excesses.

The calculation of nuclei and the EOS of nuclear matter from the same underlying interaction is one of the most challenging problems for many-body nuclear physics, and to date no completely satisfactory solution is available. The main reason is the nonperturbative nature of realistic nuclear forces, even when soft nucleon-nucleon interactions are employed. The one-pion exchange components induce strong many-body correlations with associated strong spin-isospin dependence.

Available nucleon-nucleon (*NN*) forces can fit scattering data with very high precision, with $\chi^2 \sim 1$ per data point. Accurate nuclear *NN* potentials include Argonne AV18 [1], CD-Bonn [2], and several forms of chiral forces derived within the chiral effective field theory (see, for example, Ref. [3]). The *NN* interactions are typically combined with three-body forces in such a way that the different nuclear Hamiltonians describe very accurately properties of light nuclei [4,5], medium nuclei [6,7], and homogeneous neutron matter [8–10].

Several many-body methods have been developed to accurately solve for the ground-state of light nuclei with realistic interactions. These include Green's function Monte Carlo (GFMC) [11], methods based on basis expansions, i.e., no core shell model [12], no core full configuration [13], hyperspherical harmonics [14], and others similar. The coupled cluster [15], the self-consistent Green's function [16] (SCGF), and the in-medium similarity renormalization group (SRG) [17] methods are useful to study medium nuclei. Other approaches are based on performing unitary transformation of the nuclear Hamiltonian with the goal of softening the nuclear interactions and have a fast convergence using perturbation theory [18]. Recently, coupled cluster methods have been extended to study nuclear matter [19,20].

Quantum Monte Carlo (QMC) methods, such as GFMC and auxiliary field diffusion Monte Carlo (AFDMC) [21], have proved to be accurate for predicting properties of nuclei up to $A = 12$ [22–24] and neutron matter [8,9]. Recently, new local versions of chiral forces have been fitted to scattering data and can be included in GFMC and AFDMC. They have been employed to study pure neutron matter [25] and light nuclei with $A = 3,4$ [26]. QMC methods, in contrast to other methods, do not rely on an expansion in basis sets or particle-hole excitations.

The AFDMC method has previously been applied to nuclear matter and medium nuclei [27,28], but the accuracy of these calculations was limited by the poor variational wave functions and time-step errors. Here we demonstrate these issues can be overcome, making the accuracy of AFDMC comparable to GFMC.

We present calculations of the EOS of symmetric and asymmetric nuclear matter using modern *NN* forces, demonstrating a quadratic dependence on the isospin asymmetry. Previous studies of asymmetric nuclear matter at zero temperature have been performed only within variational Fermi hypernetted chain–single operator chain technique [29] or Brueckner-Hartree-Fock [30] theory or by means of perturbative approaches [31]. At finite temperature, SCGF has also been employed [32]. We also show the application of AFDMC to light and medium-mass nuclei, including ^{16}O and ^{40}Ca, and discuss the extension to open-shell nuclei, with the inclusion of BCS-like [33] correlations. In the future it will also be possible to include three-nucleon interactions.

Quantum Monte Carlo simulations extract the ground-state properties of a many-body system through the evolution in

imaginary time τ of a trial wave function Ψ_T:

$$\Psi(\tau) = \exp[-(H - E_T)\tau]\Psi_T, \quad (1)$$

where E_T is a parameter that controls the normalization of the wave function, H is the Hamiltonian of the system

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} v_{ij}, \quad (2)$$

and v_{ij} is a two-body *NN* potential. In the limit of $\tau \to \infty$ the wave function $\Psi(\tau)$ converges to the lowest energy state not orthogonal to Ψ_T. AFDMC calculations use the trial wave function Ψ_T to minimize the variance of the calculation and as a constraint to control the fermion sign problem [34]. In previous AFDMC calculations highly simplified wave functions, without any tensor or other spin-isospin-dependent correlations, have been used. Such trial wave functions are inadequate to treat systems with both neutrons and protons, because the tensor interaction in the np ($T = 0$) channel is very large. The expectation value of the tensor interaction is nearly zero without tensor correlations, therefore these correlations are an essential feature of the nuclear wave function.

In addition, in most of the previous AFDMC calculations the auxiliary fields were sampled using the method described in Ref. [34]. We have found much better time-step dependence by adopting the sampling technique typically used in GFMC calculations [35]. The auxiliary fields are sampled from Gaussians, and the walker is propagated with auxiliary fields having opposite signs (we reverse the spatial moves and the spin-isospin rotations separately), and the final walker is sampled from these two or four choices according to their importance sampled weight. This method removes any time-step errors associated with higher-order derivatives of the trial wave function.

In this work we have considered the Argonne AV6′ interaction [36], and a new interaction that we call AV7′ with an additional spin-orbit term added to AV6′ to improve the phase shift fit [37]. This interaction is identical to AV8′ in pure neutron systems and is adjusted to give the best reproduction of AV8′ in the $^3S_1 - {}^3D_1$ coupled channels. The extension of AFDMC to deal with this isospin-independent spin orbit is possible without any further approximation [38]. The AV7′ force gives a much better fit to the lower partial wave nucleon-nucleon phase shifts than AV6′. In addition, the spin-isospin structure of AV7′ is the same as local chiral forces up to next-to-next-to-leading order (N^2LO), so AFDMC can be easily extended to use these chiral potentials [25,39].

We use a trial wave function of the following form:

$$\langle R,S|\Psi_T\rangle = \langle RS| \left[\prod_{i<j} f_c(r_{ij})\right] \left[1 + \sum_{i<j,p} f_p(r_{ij}) O_{ij}^p\right] |\Phi\rangle, \quad (3)$$

where the p sum is over the operators $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$, and $(3\boldsymbol{\sigma}_i \cdot \hat{r}_{ij} \boldsymbol{\sigma}_j \cdot \hat{r}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j)\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$. This wave function is not extensive and not as accurate as the one used in GFMC for light nuclei [35], but it has substantial overlap with the tensor components, unlike the simple wave functions used in previous AFDMC calculations. The major drawback of the GFMC wave functions is that it requires an exponentially growing number of operations with A, whereas the wave function of Eq. (3) requires order A^3 operations which is feasible even for large systems. The radial functions $f_p(r)$ are obtained by minimizing the two-body cluster contribution to the energy per particle of symmetric nuclear matter at saturation density, as described in Ref. [40]. All the variational parameters are determined by minimizing the variational energy of a given nucleus, following the procedure described in Ref. [41]. The large improvement of the above wave function with respect to the simpler one used in Refs. [27,28] is confirmed by the fact that the variational energies for both nuclei and symmetric nuclear matter are negative. This is not true for the simple wave functions without tensor correlations.

The mean-field wave function $\Phi(R,S) = \langle RS|\Phi\rangle$ has the proper quantum numbers and asymptotic behavior. It is a sum of Slater determinants of the form $\mathcal{A}\{\phi_\alpha(\boldsymbol{r}_i, s_i)\}$, where $\mathcal{A}$ is the antisymmetrizer operator, ϕ_α are single particle orbitals, and α are the single-particle quantum numbers. For nuclei, a sum of Slater determinants is sometimes needed to give the correct quantum numbers (π, J, T) for the nucleus of interest. The spatial orbital forms are obtained from a Hartree-Fock calculation with Skyrme forces. The form is described in Ref. [42] with the addition of the isospin. In the case of nuclear matter, the spatial parts of ϕ_α are plane waves with momenta allowed by periodic boundary conditions as described in Ref. [8]. The inclusion of BCS correlations is straightforward; the $\Phi(R,S)$ are replaced with a BCS form written as a Pfaffian as in superfluid neutron matter [43,44]. Pairing correlations are expected to be important in describing even-odd splittings in open-shell nuclei, in neutron-rich nuclei, and in nuclear matter at lower densities.

In order to demonstrate that the AFDMC results are accurate, we first present results for light nuclei where accurate GFMC calculations are available. We then show results for some medium-size nuclei and asymmetric nuclear matter. We have calculated the binding energies of ^{4}He using AV6′, AV7′, and the chiral N^2LO, and compared them with the corresponding GFMC values taken from Refs. [26,36]. As shown in Table I, all the results are in good agreement; the difference between AFDMC and GFMC is less than 0.125 MeV per nucleon. In GFMC calculations of the wave function for AV7′, the expectation value of the AV8′ Hamiltonian is within 0.1 MeV of the complete AV8′ calculation. This suggests it may be possible to treat higher-order corrections, for example, N3LO

TABLE I. Binding energies for ^{4}He using different two-body interactions and different cutoff R_0. The GFMC energies are taken from Refs. [26,36]. The Coulomb contribution has been perturbatively subtracted from GFMC results.

Hamiltonian	AFDMC	GFMC
AV6′	−27.09(3)	−26.85(2)
AV7′	−25.7(2)	−26.2(1)
N^2LO ($R_0 = 1.0$ fm)	−24.41(3)	−24.56(1)
N^2LO ($R_0 = 1.2$ fm)	−25.77(2)	−25.75(1)

TABLE II. Binding energy of ^{16}O and ^{40}Ca using Argonne *NN* forces. The experimental energies are also shown.

	AV6′	AV7′	Expt.
^{4}He	−27.09(3)	−25.7(2)	−28.295
^{16}O	−115.6(3)	−90.6(4)	−127.619
^{40}Ca	−322(2)	−209(1)	−342.051

interactions, perturbatively. Further studies with NLO and LO interactions will be the subject of another paper.

We have also calculated the energy of ^{6}Li with the AV6′ potential. The physical structure of this nucleus is complicated, and the GFMC results have been obtained including all the possible spacial and spin symmetries in *s*- and *p*-wave orbitals in the variational wave function, as well as cluster-dependent two-nucleon correlations [35]. We have implemented a much simpler variational wave function of the form of Eq. (3) using a *jj* basis. The energy obtained with AFDMC is −28.9(2) MeV compared to the −29.57(4) of GFMC (subtracting the EM contributions). Since ^{6}Li is one of the most challenging systems in which to test the accuracy of AFDMC, the results obtained with this simple wave function are very encouraging. Other light nuclei have important clustering effects, and they will require more sophisticated variational wave functions to be implemented in AFDMC.

Using the same Argonne *NN* interactions, we have calculated the ground-state energy of ^{16}O and ^{40}Ca. The results are shown in Table II. By comparing the results with the experimental data, it is clear that both *NN* Hamiltonians underbind these nuclei, as is the case of ^{4}He. A natural conclusion is that using Argonne AV6′ and AV7′ *NN* forces, the (missing) three-body force should be attractive. This will need further investigation, but it already shows interesting features. In coupled-cluster calculations, the three-body chiral force is attractive in the case of ^{16}O [45] and repulsive in ^{40}Ca [6]. Within the in-medium SRG approach, the three-body force is attractive for several nuclei from $A = 4$ to 56 [46]. Finally, SCGF calculations of oxygen, nitrogen, and fluorine isotopes indicate that the three-body force is attractive [47]. Other recent coupled-cluster results have been obtained by also including few-body nuclei when fitting the *NN* potential. In this case, the contribution required from three-body forces for medium mass nuclei seems to be very small [48].

The EOS of symmetric nuclear matter using both the Argonne AV6′ and AV7′ interactions is shown in Fig. 1. We simulated infinite matter using from 28 to 132 nucleons in a periodic box. Finite-size corrections have been included as described in Ref. [38]. For 76, 108, and 132 nucleons at $\rho = 0.16$ fm^{-3}, the results are −14.16(2), −13.91(2), and −12.98(4), respectively, compared to −14.17(2) for 28 nucleons. As expected, the energy for the larger systems is a bit higher, consistent with the fact that the trial wave function used for the path constraint is not extensive. Using the simpler wave function with spin-isospin-independent correlations gives somewhat less binding; for 28 nucleons and AV6′ we obtain $E/N = -10.77(2)$ MeV. Previous results with the simple wave function and the previous sampling method gave

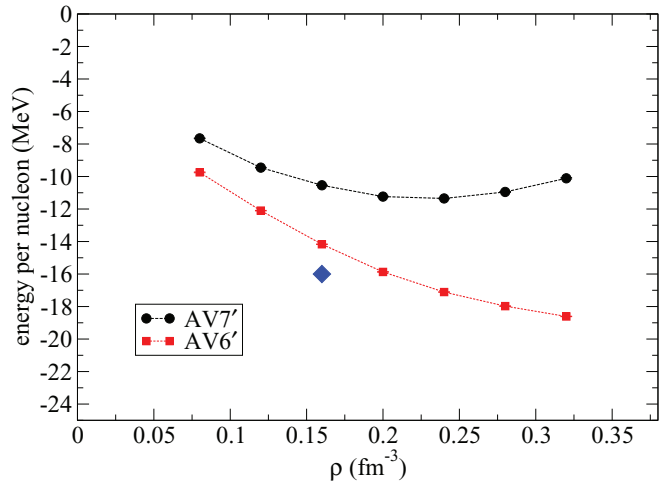

FIG. 1. (Color online) The energy per nucleon of symmetric nuclear matter obtained using the Argonne AV6′ and AV7′ interactions, see the text for details. The blue diamond indicates the hypothetical saturation point of nuclear matter.

−11.5(1) MeV [27]. The new sampling method completely removes a spurious Jastrow dependence in previous results. A critical test of quantum Monte Carlo path integral calculations is that the answers should not depend on the choice of initial trial wave function for the ground state. We have tested the accuracy of AFDMC for nuclear matter by changing the variational parameters of the spin-isospin-dependent correlations. We found that even in the case where the variational energy is not optimal, the AFDMC results are consistent within statistical errors. We have also included backflow correlations in $\Phi(R,S)$, as commonly done in liquid atomic ^{3}He [49,50] and the electron gas [51]. Introducing these backflow correlations produces the same AFDMC energies within statistical error bars.

As is clear from Fig. 1, the two different Argonne *NN* potentials give quite different results, in particular, different saturation densities, since the AV6′ and AV7′ interactions have different nucleon-nucleon phase shifts [37]. Compared with the saturation energy at $\rho = 0.16$ fm^{-3} extracted from heavy nuclei, it is clear that both *NN* Hamiltonians underbind nuclear matter. This is consistent with the results of ^{16}O and ^{40}Ca shown in Table II. The spin (isospin) structure of Argonne AV7′ is the same as local chiral forces of Ref. [25]; their implementation in the AFDMC method is straightforward. Some preliminary calculations show that, using N^{2}LO with different cutoffs, the spread of the energy of nuclear matter is similar to the difference between AV6′ and AV7′. A detailed analysis of the EOS calculated using chiral forces will be the performed in a future work.

We also report the energy of isospin-asymmetric nuclear matter at $\rho = 0.16$ fm^{-3} using the AV6′ interaction. We performed simulations using different combinations of neutrons and protons, listed in Fig. 2, filling closed shells of the discretized momenta. Corrections for the finite-size effects due to the interaction are included as described in Ref. [38]. We have corrected the AFDMC energies by subtracting from

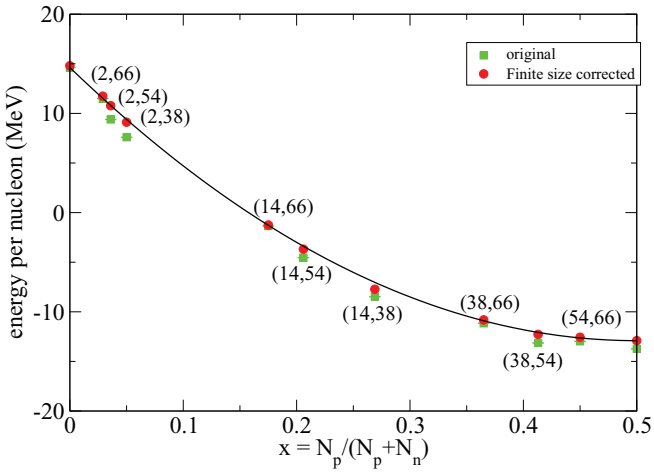

FIG. 2. (Color online) Energy per nucleon of isospin asymmetric nuclear matter calculated using the AV6′ potential as a function of the proton concentration. Green squares represent the AFDMC results and red circles the ones in which finite-size corrections are included. The numbers in parenthesis indicate the number of protons and neutrons considered in the simulations.

the AFDMC results the term

$$\delta E(\rho) = E_0(N_n, N_p, \rho) - E_{FG}(p, \rho), \tag{4}$$

where E_0 is the energy of noninteracting N_n neutrons and N_p protons in the same simulation box and E_{FG} is the energy in the thermodynamic limit at the same isospin polarization p, i.e., $E_{FG}(p,\rho) = E_{FG}(\rho)[(1+p)^{5/3} + (1-p)^{5/3}]/2$. This strategy has been successfully applied to study strongly interacting polarized Fermi liquids [52–54].

From Fig. 2 we see that our results agree with the quadratic behavior of the energy as a function of the isospin-asymmetry obtained by simply interpolating the results for $x = 0$ (pure neutron matter) and $x = 0.5$ (symmetric nuclear matter). We do not expect that using the AV7′ interaction the quadratic behavior of the energy as a function of the asymmetry would change. However, pairing correlations might play an important role, especially at lower densities.

Clearly it is important to include three-nucleon interactions in AFDMC. For pure neutron systems, three-body forces can be included exactly in the propagator because the spin-isospin operators reduce to a quadratic form in the spin [38]. In the case of nuclei and nuclear matter, the full three-body force cannot yet be included in the propagator. However, it is possible to use a simplified form of the three-body force compatible with standard AFDMC and calculate the difference from the full three-body potential perturbatively. This strategy has been extensively tested in GFMC calculations [35]. Another approach consists of reducing the three-body potential to a $V_2(\rho)$ density-dependent force, as done in Ref. [55], and perturbatively computing the difference $[V_2(\rho) - V_3]$.

In conclusion, we have presented an AFDMC method extended to *NN* forces that include spin-orbit terms, along with a significantly improved variational wave function and propagation technique. Since the forces have the same spin-isospin operatorial structure of local chiral forces at N^{2}LO, the extension of the AFDMC to chiral forces is straightforward, similar to what has been done for pure neutron matter [25,39]. We have also presented the a quantum Monte Carlo calculation of asymmetric nuclear matter using bare *NN* nuclear interactions, showing that at saturation density the energy per particle follows the often assumed quadratic behavior as a function of isospin asymmetry. This work paves the way for a systematic study of the structure of medium mass nuclei, neutron-rich nuclei, and nuclear matter using both Argonne and chiral forces with unprecedented accuracy.

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