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

S. Gandolfi,[1] A. Lovato,[2,3] J. Carlson,[1] and Kevin E. Schmidt[4]

[1] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, 87545*
[2] *Argonne Leadership Computing Facility, Argonne National Laboratory, Argonne, IL 60439*
[3] *Physics Division, Argonne National Laboratory, Argonne, IL 60439*
[4] *Department of Physics, Arizona State University, Tempe, AZ 85287, USA*

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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 forces, including a new Argonne version that has the same spin/isospin structure as local chiral forces at next-to-next-to-leading order (N2LO). The calculations are performed using Auxiliary Field Diffusion Monte Carlo (AFDMC) combined with an improved variational wave function. We show that 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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The knowledge of the equation of state (EOS) of nuclear matter, particularly with arbitrary isospin asymmetry, i.e., different proton and neutron fractions, is of fundamental importance for both nuclear physics and astrophysics. The saturation density and the energy per particle of nuclear matter can be used to test properties of finite nuclear systems extrapolated to the thermodynamic limit. Moreover, the study of the EOS of asymmetric matter allows for the understanding of the behavior of the isospin asymmetry energy, i.e., the "symmetry energy", and for constraining the bulk properties of nuclear density functionals, which are often used to predict the properties of heavy nuclei and nuclei with large neutron excesses. Experimentally accessing the properties of such nuclei constitutes a formidable task; however, they are needed to understand the observed abundances of the elements, their production in r-process nucleosynthesis in supernovae, and the properties of exotic neutron-rich nuclei found in the crust of neutron stars.

The calculation of the EOS of nuclear matter 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 non-perturbative nature of realistic nuclear forces, even when soft nucleon-nucleon interactions are employed. The repulsive core and the strong tensor components induce strong many-body correlations. Because of strong spin-isospin dependent correlations and the large number of particles, the calculation of asymmetric nuclear matter properties is more difficult than for pure neutron matter or for light nuclei.

The latest generation of modern 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 [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 interactions fit to the NN scattering data. These include the 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 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 methods, such as GFMC and the Auxiliary Field Diffusion Monte Carlo [21] (AFDMC), 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]. The AFDMC method has been also employed for studying nuclear matter and medium nuclei [27, 28], but the accuracy of these calculations was limited by the poor variational wave functions and numerical issues arising from time-step errors. In this work we show that the limitations associated with both 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. Because most previous methods have only calculated symmetric nuclear matter and/or neutron matter EOS, often a quadratic dependence of the energy on the isospin asymmetry has been assumed. Studies of asymmetric nuclear matter at zero temperature have been performed only within variational Fermi Hypernetted Chain/Single Operator Chain technique [29], Brueckner-Hartree-Fock [30] theory or by means of perturbative approaches [31]. At finite temperature, SCGF has also been employed [32].

In this work we present Quantum Monte Carlo calculations of asymmetric nuclear matter at saturation density, and demonstrate the quadratic dependence of the isospin asymmetry energy. 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. We will finally introduce a technique suitable to include three-body forces in future AFDMC calculations, that can in principle be included in other methods as well.

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:

$$\Psi(\tau) = \exp[-(H - E_T)\tau]\Psi_T \tag{1}$$

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

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

and v_{ij} 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 not fully adequate to treat systems with both neutrons and protons. The reason is that the tensor interaction in the np ($T = 0$) channel is very large. It can be shown that the expectation value of the tensor component of the NN potential is nearly zero if the tensor correlations are not included in the variational wave function. Therefore, those 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. Within this technique, the auxiliary fields are sampled from real gaussians, and a walker is propagated according to the 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 gradients of the trial wave function.

In this work we have considered the Argonne AV6′ interaction [35], and a new interaction that we call AV7′ with an additional spin-orbit term added to AV6′ to improve the phase shift fit [36]. 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 [37]. (The isospin-dependent spin-orbit either would need to be included perturbatively, or by more sophisticated sampling methods not described here). 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^{2}LO), so that AFDMC can be easily extended to use chiral potentials of the form of Ref. [25, 38].

In order to improve the algorithm and avoid the aforementioned limitations associated with the simple trial wave functions, we have implemented a trial wave function including tensor correlations:

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

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 [39], 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 their evaluation requires a number of operations exponentially growing with A. Instead, the evaluation of the wave function of Eq. (3) requires order A^3 operations so that its calculation 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. Its general form is given by 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 that have the proper asymptotic behavior depending on the system, and α are the single-particle quantum numbers. For the case of nuclei, a sum of many 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 fitting the simulation box as described in Ref. [8]. Note that the inclusion of BCS correlations is straightforward; it is easy to replace $\Phi(R,S)$ 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.

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 I. Binding energies for ^{4}He using different two-body interactions. The GFMC energies are taken from Refs. [26, 35]. The Coulomb contribution has been perturbatively subtracted from GFMC results.

In order to demonstrate that our results are accurate for asymmetric matter, we first show some results for light nuclei where accurate GFMC calculations are available. We then show results for some medium-size nuclei with comparison to experiment. Having demonstrated the accuracy of the AFDMC method with the wave function of Eq. 3, we show results for asymmetric nuclear matter.

We have calculated the binding energies of ^{4}He using AV6′, AV7′, and the chiral N^2LO, and compared those with the corresponding GFMC values taken from Ref. [26, 35]. 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. We have also compared GFMC and AFDMC results for ^{4}He using chiral forces at NLO and LO, getting a similar agreement; these study will be the subject of a following paper.

We have also calculated the energy of ^{6}Li using the AV6′ potential. The physical structure of this nucleus is complicated, and the results using GFMC have been obtained by including all the possible spacial/spin symmetries in s- and p-wave orbitals in the variational wave function, as well as cluster-dependent two-nucleon correlations [39]. 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 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 calculations, beyond the scope of this paper.

	AV6′	AV7′	exp
^{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

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

Using the same Argonne NN forces, 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. We may conclude that using Argonne AV6′ and AV7′ NN forces, the (missing) three-body force should be attractive. This will need further investigation, but already shows interesting features. Using chiral forces in coupled cluster calculations, the three-body is attractive in the case of ^{16}O [45], and repulsive in ^{40}Ca [46]. Within in-medium SRG approach, the three-body force is attractive for several nuclei from A=4 to 56 [47]. Finally, SCGF calculations of oxygen, nitrogen and fluorine isotopes indicate that the three-body force is attractive [48]. 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 [49].

We have also calculated the EOS of symmetric nuclear matter using both the Argonne AV6′ and AV7′ interactions, with results shown in Fig. 1. We simulated infinite matter using 28 nucleons in a periodic box. Finite size corrections due to the truncation of the pairwise potential to distances equal to $L/2$ (L is the box size) have been included as described in Ref. [37]. We have also calculated the energy given by 76, 108, and 132 nucleons at ρ=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 higher, consistent with the fact that the trial wave function used for the path constraint is not extensive.

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

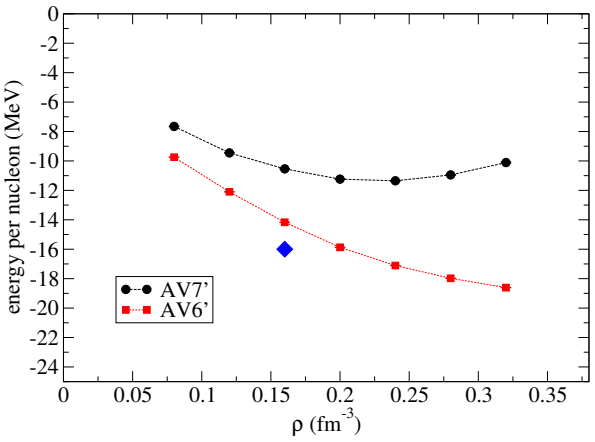

FIG. 1. (color online) The energy per nucleon of symmetric nuclear matter obtained using the Argonne AV6′ and AV7′ interactions, see the text for details. The blue diamond indicates the hypothetical saturation point of nuclear matter.

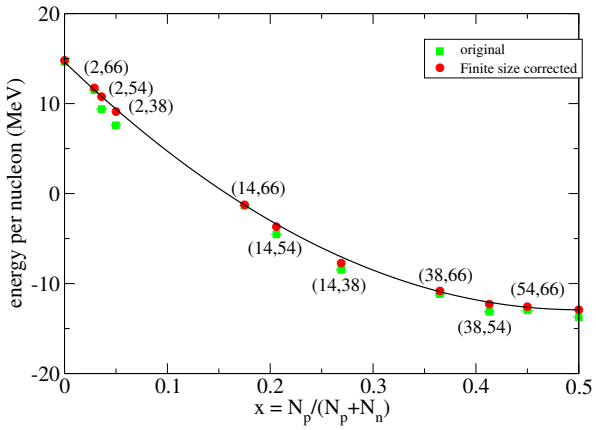

FIG. 2. (color online) Energy per nucleon of isospin asymmetric nuclear matter calculated using AV6′ potential as a function of the proton concentration. Green squares represent the AFDMC results and red circles the ones in which finite size corrections are included. The numbers in parenthesis indicate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

in the case where the VMC energy is not optimal, the AFDMC results are consistent within statistical errors. We have included backflow correlations in $\Phi(R,S)$, as commonly done in liquid atomic ^{3}He[50, 51] and the electron gas[52], where it is motivated by the repulsive part of the two-body potential. We have checked that backflow correlations produce 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. This is due to the fact that the AV6′ and AV7′ interactions have different nucleon-nucleon phase shifts [36]. In any case, comparing with the energy at ρ=0.16 fm^{-3} extracted from heavy nuclei, (in the figure the blue diamond correspond to the saturation point), 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 have calculated the energy of isospin-asymmetric nuclear matter at ρ=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 discretised momentum. Corrections for the finite size effects due to the interaction are included as described in [37]. In order to alleviate finite size effects arising from the kinetic energy, we have corrected the AFDMC energies by subtracting from the AFDMC results the term

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

In the previous equation, E_0 is the energy of non-interacting 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, 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 [53–55].

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, and will be included and addressed in future works. It will be interesting to see if the inclusion of superfluid pairing alters these results.

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 [37]. 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 as a perturbation. This strategy has been extensively tested in GFMC calculations [39]. Another approach consists in reducing the three-body

potential to a $V_2(\rho)$ density dependent force as done in Ref. [56], and perturbatively compute the difference $[V_2(\rho) - V_3]$.

In conclusion, we have presented a new AFDMC method extended to NN forces that include spin-orbit terms, along with a significantly improved variational wave function and improved 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 use them is straightforward, similar to what has been done for pure neutron matter [25, 38]. We have also presented the first 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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