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GFMC studies of low-density neutron matter

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Abstract. Green's function Monte Carlo methods are used to provide benchmarks for studies of low-density neutron matter. The zero-temperature equation of state and pair correlation functions are studied for the AV8′ NN interaction model, and for an idealized model comprised of neutrons with a short-range interaction and an arbitrarily large (negative) scattering length. For this idealized problem the equation of state is a constant multiplied by the Fermi-gas energy, this constant is found to be nearly 1/2. Similar ratios are found for realistic NN interactions.

PACS. 26.60.+c Nuclear matter aspects of neutron stars – 21.65.+f Nuclear matter – 21.30.-x Nuclear forces

1 Introduction

Low-density neutron matter is an interesting many-body problem because of the very large s-wave scattering length in the spin-0 channel, and the complications that arise from the short-range repulsion and the tensor and the $L \cdot S$ components in the nucleon-nucleon interaction. Physically the ground state of neutron matter can be important in characterizing the properties of neutron-rich nuclei and the low-density region of neutron stars.

The properties of neutron matter, even at low densities, are more difficult to determine than nuclear matter, since the latter can be determined near equilibrium densities from the properties of nuclei. Microscopic many-body theories, combined with realistic interaction models, offer the prospect of accurate determinations of the properties of neutron matter. It is hoped that these calculations will prove useful, for example, in calculations of effective interactions and energy-density functionals for neutron and neutron-rich matter [1].

Traditionally, neutron matter has been studied in Brueckner [2,3] or variational [4,5] theories. These methods have many strengths, but also some potential weaknesses. In particular, it can be difficult to characterize the importance of many-body correlations. Monte Carlo methods have been very successful in treating many-body problems in other fields [6], as well as few-nucleon systems [7]. In this paper we report results of variational Monte Carlo (VMC) and Green's function Monte Carlo (GFMC) calculations of neutron matter, using the same methods employed to reproduce the binding energy of light nuclei. Promising advances have also been made combining Auxiliary Field and Diffusion Monte Carlo methods [8] for the studies of neutron and nuclear matter. While the standard method is limited to small numbers of particles, it has proven very accurate in studies of light nuclei, and can provide valuable benchmarks. In particular, these methods can be used to study the correlation functions, which in traditional variational studies can differ greatly with only fairly modest effects in the total energy.

We have also used Monte Carlo methods to study an idealized case of neutrons interacting via a short-range potential with an infinite scattering length. This problem was proposed by Bertsch, and contains many of the interesting features of realistic neutron matter. It should also be of interest in studies of Fermi atomic gases, where attempts are being made to study a system at very low temperature. Dimensional arguments show that in this limit the ground-state energy of such a system as a function of energy must be a fixed fraction of the Fermi-gas energy. Here we determine this fraction and study the resulting pair distribution functions.

2 Interaction

Realistic models of the nuclear Hamiltonian generally take the form

$$T = H + V = -\frac{\hbar^2}{2m}\nabla^2 + V_{ij} + V_{ijk}, \qquad (1)$$

where the nucleon-nucleon (NN) interaction contains one-pion exchange at long range, intermediate-range terms characterized by terms of two-pion exchange range, and

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a phenomenological short-range interaction. Examples of modern interactions that fit the NN scattering data with $\chi^2 \approx 1$ are the Reid-93, Nijmegen II [9], Bonn-CD [10] and Argonne v_{18} (AV18) [11] interactions.

Each of these interactions have 6 momentum-independent terms, with operator forms constructed from $1, \sigma_i \cdot \sigma_j, S_{ij}$, and $\tau_i \cdot \tau_j$. Simplified NN interaction models with these terms alone are called v_6 interactions, those which also include $L \cdot S$ and $L \cdot S \tau_i \cdot \tau_j$ are called v_8 models. These terms are the dominant terms in the NN interaction; the calculations reported here are for the AV8′ NN interaction model obtained from the AV18 interaction. The prime indicates that the potential has been refit in the lowest partial waves, and is not a simple truncation of AV18.

Realistic interaction models include additional terms proportional to the square of the momentum, these are required to get an accurate representation of all the partial waves. Different models of the NN interaction may have different (local or non-local) representations of the one-pion exchange potential. These different representations are related by unitary transformations, and require different two-nucleon currents as well as different three-nucleon interactions the unitary transformations.

Three-nucleon interactions are also required to fit the binding energy of light nuclei. The isospin dependence of the three-nucleon interaction can play an important role in the properties of neutron matter. This has been studied extensively in light nuclei, where the Illinois TNI models have been fit to nuclear levels up to $A = 8$ [7], and recent calculations include up to mass 10 [12].

Relativistic effects can also be expected to play a role, particularly at higher densities [13]. In general, the two-nucleon interaction must depend not only upon the relative momenta of the two nucleons $\mathbf{p} = \mathbf{p}_i - \mathbf{p}_j$, but on the total momentum $\mathbf{P} = \mathbf{p}_i + \mathbf{p}_j$. The lowest-order terms in $\mathbf{P}^2$ can be obtained directly from the CM frame NN interaction, as shown by Foldy and Friar [14]. This boost interaction is repulsive, and has been estimated to contribute approximately 2 MeV in the alpha-particle, and raises the nuclear-matter saturation energy by approximately 4 MeV per nucleon. The density dependence of this interaction is similar to that of the short-range TNI terms in the Urbana and Argonne TNI models.

For the purposes of this study, we consider the minimal semi-realistic interaction, the AV8′. Demonstrably accurate calculations of such simple models are important in order to believe results obtained with more refined interactions. Light nuclei are under bound with this interaction, and hence one expect the energies reported here to be too high compared to a more complete calculation.

3 Methods

We compare results obtained with variational Fermi hypernetted-chain (FHNC) methods to those obtained with variational Monte Carlo (VMC) and Green's function Monte Carlo (GFMC). FHNC methods have been used extensively in studies of nuclear and neutron matter [13,5]. In its simplest form, FHNC is used to calculate the expectation value of the energy:

$$\langle H \rangle = \frac{\langle \Psi_\mathrm{T} | H | \Psi_\mathrm{T} \rangle}{\langle \Psi_\mathrm{T} | \Psi_\mathrm{T} \rangle}, \tag{2}$$

with a specific form of the trial wave function:

$$\Psi_\mathrm{T} = \mathcal{S}\left[\prod_{i<j} F_{ij}\right] |\Phi\rangle , \tag{3}$$

where F_{ij} is a spin-dependent pair correlation function, and Φ is the uncorrelated Fermi-gas wave function. The trial or variational wave function is then optimized by minimizing the energy as a function of a set of parameters used to construct the pair correlation functions F_{ij}.

FHNC provides only an approximate evaluation of the energy for this wave function. In the standard approach, three-nucleon terms and higher are treated approximately. Recently, this has been improved by the Urbana group with an exact treatment of all three-nucleon terms.

We test the approximate treatment of these terms by performing a variational Monte Carlo calculation including an exact evaluation of many-body terms. The difference between the VMC and FHNC results then provide an estimate of the importance of the approximations made in FHNC calculations.

In addition, we use Green's function Monte Carlo methods to sample the exact ground-state wave function:

$$|\Psi_0\rangle = \exp[-H\tau] |\Psi_\mathrm{T}\rangle . \tag{4}$$

This method provides a way of including correlations beyond the simple Jastrow type, and is in principle exact in the limit $\tau \to \infty$. This limit can be difficult to reach in some cases because of the fermion sign problem. Here we used a constrained path approach which provides a constraint on the sums over the paths included in the path integral sampled to produce the ground-state wave function [15]. As a test, the constraint is then removed and the ground-state energy calculated as a function of the unconstrained propagation time τ [16]. This method has been studied extensively in few-nucleon systems, and the difference between variational and GFMC results can be quite significant.

The Monte Carlo methods employed in this study are limited to systems of only a few nucleons as they sum explicitly over the 2^A spin states of the system. Therefore, the Monte Carlo calculations are performed for 14 neutrons in periodic boundary conditions. The volume of the periodic cube is adjusted to vary the density: $\rho = 14/L^3$. The potential is truncated at $L/2$ to simplify comparisons between integral equation and Monte Carlo methods.

The uncorrelated Fermi-gas wave function with these boundary conditions occupies states of momentum $\mathbf{k} = 0, \pm k_b \hat{\mathbf{x}}, \pm k_b \hat{\mathbf{y}}$, and $\pm k_b \hat{\mathbf{z}}$, where $k_b = 2\pi/L$. The kinetic energy of this state is $5.82 \rho^{2/3} \hbar^2/2m$ compared to the infinite-volume limit of $5.74 \rho^{2/3} \hbar^2/2m$.

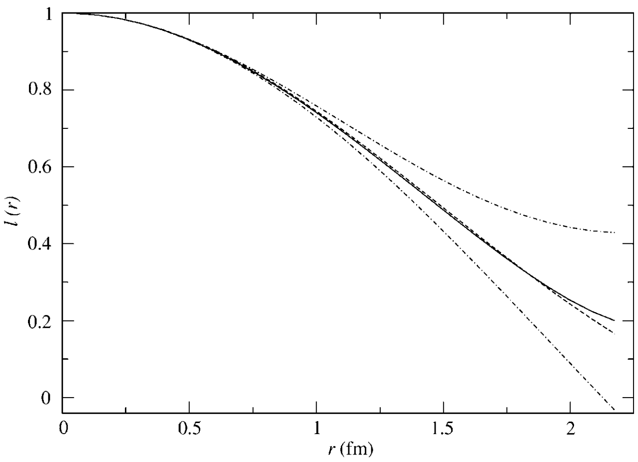

Fig. 1. Slater function l for 14 particles in periodic boundary conditions along the axes and diagonal of the simulation cube (top and bottom dash-dotted lines) compared to the angle-averaged result in the cube (solid line) and the infinite-volume limit (dashed line).

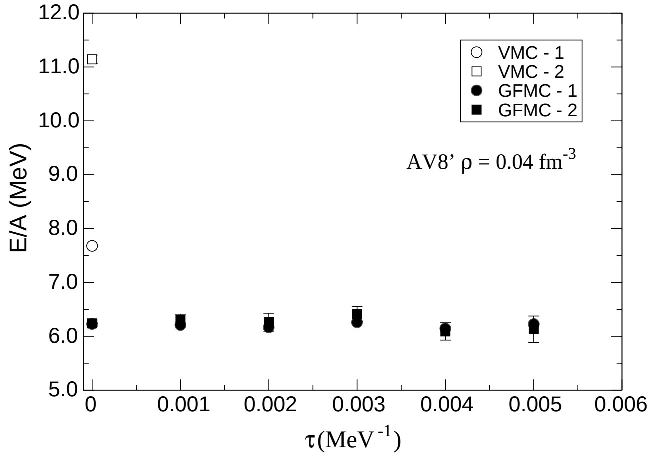

Fig. 2. VMC and GFMC results at $\rho = 0.04$ fm^{-3}. Open symbols are VMC results obtained with two different trial wave functions, GFMC results with constraint are shown at $\tau = 0$ as solid symbols, and without constraint as a function of τ.

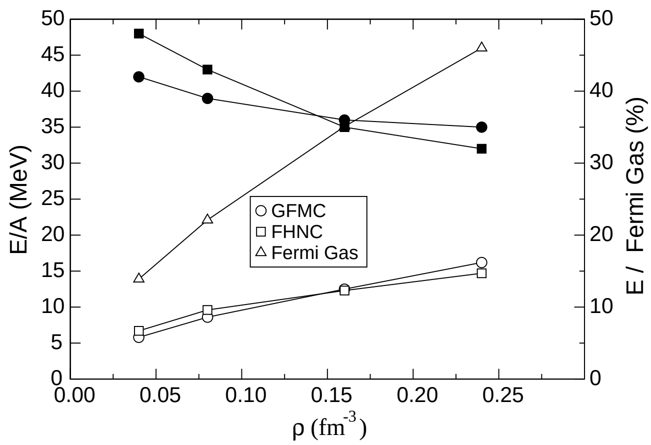

Fig. 3. Energy *vs.* density (ρ) for FHNC and GFMC calculations and the Fermi-gas energy. Open symbols are plotted *vs.* absolute energy (left scale), solid symbols are plotted as a fraction of the Fermi-gas energy (right scale).

The free finite-volume one-body density matrix is compared to the infinite-volume limit in fig. 1. The density matrix is:

$$\rho(\mathbf{r}', \mathbf{r}) = \sum_{i=1,N} \exp[-ik_i \cdot (\mathbf{r} - \mathbf{r}')] = \rho l(|\mathbf{r} - \mathbf{r}'|). \qquad (5)$$

Though in specific directions the density matrix is quite different from the infinite-volume limit, the angle-averaged density matrix is in fact quite similar to the complete non-interacting result.

4 AV8 results

Variational and FHNC calculations have been performed for the same wave functions at densities of 0.04, 0.08, 0.16, and 0.24 fm^{-3}. The wave functions used have short-range correlations, even compared to the $L/2$ restriction required by periodic boundary conditions. For example, at $\rho = 0.04$, $L/2 = 3.53$ fm while the correlation lengths are taken to be 1.76 fm. The energy obtained was within 0.25 MeV$/A$ of that obtained by the optimum long-range correlations typically used in FHNC studies. For these short-range correlations, the cluster expansion works extremely well and excellent agreement is obtained between VMC and FHNC results. The 3-body cluster contributions in such states are quite small; studies with longer correlation lengths are in progress. In FHNC, the energy depends only weakly upon the correlation length, and hence the energy must be evaluated quite accurately in order to determine the correct NN correlations in matter. The exact treatment of 3-body clusters should be quite valuable in this regard. Long-range correlations can have important effects in the electroweak response of the system, particularly at low momentum transfer.

We have also calculated the ground-state energy using GFMC methods starting with the variational wave functions. The energy as a function of imaginary time for two different initial states is shown in fig. 2. While the VMC results are quite different, the GFMC results are in good agreement with each other. The GFMC points shown at $\tau = 0$ are the results of (approximate) constrained path calculations, the energy is then plotted as a function of the imaginary time after the constraint is removed. Results appear to be well converged and independent of the trial wave function. Results at moderate densities are similar, though by $\rho = 0.24$ fm^{-3} the fermion sign problem is much more severe.

In fig. 3 we compare the ground-state energy as a function of density for the FHNC and GFMC results. At low densities the GFMC results are somewhat lower (10%) than the FHNC results, presumably due to three- and more-nucleon correlations absent in the FHNC wave function. These correlations have been found to play a significant role in light nuclei. At higher densities the curves cross, and the FHNC energy is slightly lower than the

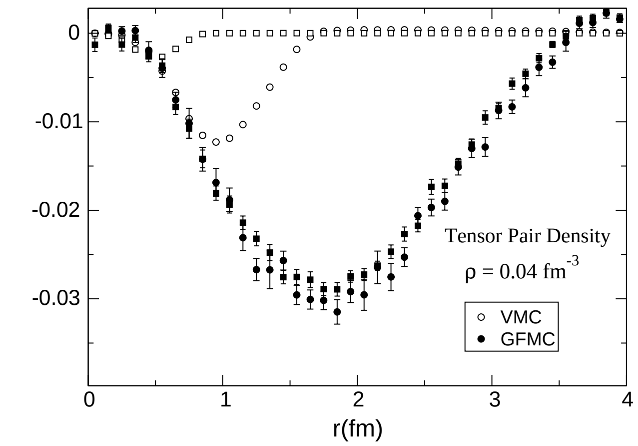

Fig. 4. Tensor correlation function at $\rho = 0.04$ fm^{-3}, VMC (open symbols) and GFMC (filled symbols). Calculations with two different trial states are indicated as circles and squares.

GFMC result at 0.24 fm^{-3}. This may be due to inaccuracies in the FHNC calculations for three- or more-nucleon clusters, or to difficulties with calculating fermions at high densities.

We have also computed pair distribution functions in neutron matter. The initial trial states, as discussed above, have very small correlation lengths. Even in such cases, though, the GFMC finds the long-distance correlations present in the true ground state. Here we present only the results for the tensor correlation function, see fig. 4. Again results obtained with two different trial wave functions are consistent with each other. The GFMC correlations are long range and similar in shape to those found in infinite-volume limit FHNC calculations. Further tests including trial states with longer-range correlations are being pursued.

5 Simple model

We have also performed studies of a very simple model of neutron matter, first proposed by George Bertsch [17]. In this model, we consider an interaction which has an infinite (negative) scattering length, and take the limit where the range of the interaction goes to zero. This is an appropriate description for low-density neutron matter, where the real scattering length is much larger than the interparticle separation. It may also be used to describe trapped atomic Fermi gases, where the interaction can be tuned using Feshbach resonances.

It is clear that the ground-state energy of such a system must be a fraction of the Fermi-gas energy, where the fraction is a constant independent of energy. Also clearly there must be very strong singlet pairing arising from the strength of the interaction. The model has many similarities to real neutron matter at low densities because the nn scattering length (-18.5 fm) is much larger than the average particle separation $2r_0$ except at extremely small densities: $\rho = 4/3\pi r_0^3$. Even at $\rho = 0.02$ fm^{-3}, $r_0 \approx 2.3$ fm, and $2r_0$ is still much smaller than the scattering length. Simultaneously, $2r_0$ is larger than the range of the real NN interaction.

We have constructed a short-range potential with infinite scattering length, and then used VMC and GFMC methods to calculate the energy and pair correlation functions. This is a particularly simple case because the interaction can be assumed to be spin independent with zero range. Therefore, standard spin-independent VMC and GFMC methods can be used. Of course only $S = 0$ pairs interact, the interaction in the $S = 1$ channel is forbidden by the Pauli principle.

It is possible to use VMC and GFMC methods to study this problem in the exact zero-range limit, and this is currently being pursued. VMC is fairly straightforward as long as the trial wave function being considered has the correct form as the separation between spin singlet pairs goes to zero. For GFMC, one only needs the exact 2-body propagator ($\langle \mathbf{r}'_{ij} | \exp[-H_{ij}\tau] | \mathbf{r}_{ij} \rangle$) between neutrons can be written down analytically for this problem, and used in the sampling of the paths.

Here we take a simpler approach and use a Gaussian potential of small range tuned to give an infinite scattering length:

$$V(r) = V_0 \exp[-(r_{ij}/r_0)^2], \qquad (6)$$

where we have chosen $r_0 = 0.5$ fm. To maintain the limit of an infinite scattering length, the strength V_0 must go to infinity as $r_0 \to 0$, but the volume integral of the potential goes to zero. Corrections to these results are expected to be small because three-body contributions will necessarily involve a p-wave between particles, which will be very small inside the range of this interaction. The effect of finite effective ranges in the potential remain to be studied.

We have solved this problem in two different cases, first for 14 neutrons at a density of 0.04 fm^{-3}, and for 54 neutrons at a density of 0.02 fm^{-3}. The density is only relevant because we have used a finite-range potential. For 14 neutrons, we can insert an $S = 0$ projection operator in the interaction and the pair correlation operator F_{ij} to eliminate the interactions and correlations between all p-wave pairs. For 54 particles this projection operator would require the use of Auxiliary Field Diffusion Monte Carlo methods, and hence we use the spin-independent potential above. In the limit $r_0 \to 0$ these two problems are identical.

For 14 neutrons at $\rho = 0.04$ fm^{-3}, we find a variational upper bound of $E/A = 8.36 \pm 0.05$ MeV. For free particles with these same boundary conditions, $E/A = 14.13$ MeV, and hence $E(\mathrm{VMC})/E(\mathrm{FG}) \approx 0.60$. For the same interaction, GFMC with a constraint yields an energy of 7.06 ± 0.08 MeV, so $E(\mathrm{GFMC})/E(\mathrm{FG}) = 0.50 \pm 0.06$. Relaxing the constraint produced no apparent decrease in energy. GFMC calculations for 54 particles at $\rho = 0.02$ fm^{-3} yields an upper-bound fixed-node result of $E(\mathrm{GFMC})/E(\mathrm{FG}) = 0.505 \pm 0.010$, where we have again divided by the finite-volume 54-particle Fermi-gas energy $E(\mathrm{FG}) = 8.444$ MeV. Relaxing the fixed-node condition up to $\tau = 0.005$ MeV^{-1} did not produce a statistically significant lowering of the energy.

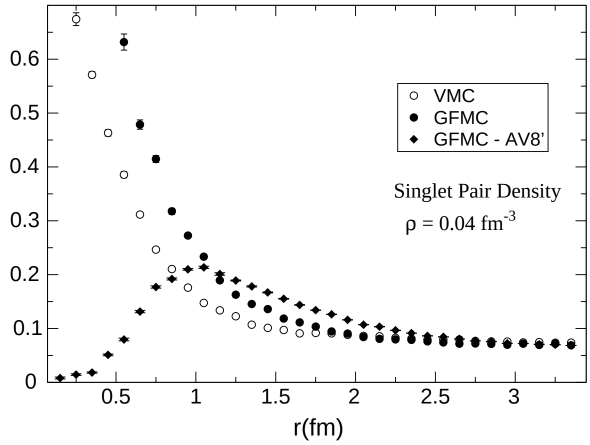

Fig. 5. Spin singlet pair densities for the short-range potential, VMC (open circles) and GFMC (closed circles) results. For comparison, results at the same density for the AV8′ NN interaction are shown.

Unless these wave functions are orthogonal (or nearly so) to the true ground state, the energy per particle is approximately 1/2 the Fermi-gas energy. Clearly, there is strong spin-zero pairing in this simple model, in fig. 5 we plot the spin singlet pair distribution function. The radial shape is different from the realistic interaction due to the short-range repulsion, but both are enhanced significantly over the free-particle result. The spin triplet channel shows no such enhancement.

6 Conclusion

We have calculated the properties of neutron matter at low density using variational and Green's function Monte Carlo methods in order to provide a benchmark for other types of calculations. The particular methods used here are limited in that they can treat only small numbers of particles, but they have proven to be very accurate. Auxiliary Field Diffusion Monte Carlo methods are potentially the best treatment.

We have compared the results with FHNC calculations, and found fairly modest differences in the results ($\approx 10\%$). The ground-state energy at small densities are roughly 40% of the Fermi-gas energy, in rough agreement with the 50% found for the simple short-range interaction model. GFMC calculations of the pair correlation functions confirm the long-range spin-dependent correlations found in FHNC calculations, even starting from trial states in which they are absent.

Of course it would be extremely interesting to study additional properties of the system, including spin susceptibility, superfluidity, response and finite-temperature properties. Of course studies with realistic interactions, adjusted to reproduce both the properties of light nuclei and bulk properties of matter, are crucial. It will also be important to study simple models such as those described here to gain a simpler understanding of the important mechanisms in such Fermi systems. There is every reason to be optimistic that both the computational methods and our understanding of these systems will advance rapidly over the next few years.

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