Quantum Monte Carlo calculations of symmetric nuclear matter

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We present an accurate numerical study of the equation of state of nuclear matter based on realistic nucleon–nucleon interactions by means of Auxiliary Field Diffusion Monte Carlo (AFDMC) calculations. The AFDMC method samples the spin and isospin degrees of freedom allowing for quantum simulations of large nucleonic systems and represents an important step forward towards a quantitative understanding of problems in nuclear structure and astrophysics.

1. INTRODUCTION

The knowledge of the properties of symmetric and asymmetric nuclear matter, is one of the main ingredients of the equations predicting the structure, the dynamics and the evolution of stars, in particular during their last stages, when they become ultra–dense neutron stars. The large variety of available results, partly due to the use of many different approximations, and partly to the limited knowledge of the nucleon–nucleon interaction, lead to different interpretations and hypothesis. Depending on the model used, the density of nuclear matter in the inner shells can reach up to 9 times the core density of stable nuclei, $\rho_0 = 0.16 \text{ fm}^{-3}$, or be limited to 4-5 times $\rho_0$.

One important step towards the understanding of these astrophysical problems is the study of the symmetric nuclear matter, related to the various model NN interactions available. While considerable advances have been made,\textsuperscript{2,3} it is still impossible to understand how different results de-
pend on the model interaction used rather than on the particular approxi-

Therefore, it is not possible to draw conclusions when comparing with
astronomical observations. However, the recent success in predicting the
properties of light nuclei gives us some confidence that the non–relativistic
description of nuclear matter based on effective potentials fitted to repro-
duce NN data and the binding energy of light nuclei can be reliable enough.
The main feature of such nucleon–nucleon interactions, besides the short
range repulsion, is the explicit dependence on the relative quantum state
of the nucleons which can be described using spin and isospin, angular
momentum, spin–orbit, and tensor operators.\textsuperscript{4}

Properties of light nuclei ($A \leq 6$) can be efficiently computed with high
accuracy using modern few–body techniques\textsuperscript{5–7} or with the ab initio no-core
nuclear shell model (with $A \leq 12$).\textsuperscript{8} Quantum Monte Carlo techniques based
on recasting the Schroedinger equation into a diffusion equation (Diffusion
Monte Carlo or Green’s Function Monte Carlo), allowed for performing
calculations up to $A \leq 12$.\textsuperscript{9,10} However, the computational resources needed
for such simulations are very large, because of the summation over all the
possible states necessary to evaluate the terms of the Hamiltonian with
a quadratic dependence on spin and isospin. The number of such terms,
and the CPU time needed to calculate them, grows exponentially with the
number of nucleons; $^{12}\text{C}$\textsuperscript{9} or 14 neutrons\textsuperscript{11} is the limit for the currently
available computational resources.

Since the spatial degrees of freedom are already sampled, one would like
to replace the sum over the spin–isospin states with an efficient sampling
method. The simulation of symmetric nuclear matter requires a minimum
of 28 nucleons in a box replicated in space (7 nucleons for each spin–isospin
state) to obtain a wave function with closed shells of momenta, and this is
out of the reach of the standard Quantum Monte Carlo methods.

Recently\textsuperscript{12} we shown that the spin–isospin is efficiently sampled by using
the Auxiliary Field Diffusion Monte Carlo method,\textsuperscript{13} which is based on the
use of auxiliary variables to linearize the quadratic spin–isospin operators of
the nuclear matter Hamiltonian, making them treatable in a diffusion Monte
Carlo scheme. Up to now it has been applied to simulate pure neutron
matter (up to 114 neutrons),\textsuperscript{14,15} and neutron drops\textsuperscript{16,17} interacting with
realistic two– plus three–body interactions.

Here we extend calculations to include isospin degrees of freedom and to
deal with the strong tensor–isospin force, responsible of the nuclear binding.
The method can readily handle an asymmetry in the number of neutron
and protons or the deformation of heavy nuclei.

2. METHOD

Auxiliary Field Diffusion Monte Carlo (AFDMC)\(^{13}\) is an extension of the standard Diffusion Monte Carlo method in which the ground state of an Hamiltonian \(H\) is obtained by solving the imaginary time dependent Schrödinger equation. The solution is obtained by evolving a population of configurations of the system (“walkers”) \(X = \{R, \sigma, \tau\}\), where \(R = \{\vec{r}_1, \ldots, \vec{r}_N\}\), \(\sigma = \{\vec{\sigma}_1, \ldots, \vec{\sigma}_N\}\), and \(\tau = \{\vec{\tau}_1, \ldots, \vec{\tau}_N\}\), with \(F(X, t) = \Psi_T(X)\Psi(X, t)\), according to

\[
F(X, t) = \int dX' \frac{\Psi_T(X)}{\Psi_T(X')} G_0(X, X', t)F(X', 0) \tag{1}
\]

The function \(\Psi_T\) is a “trial” wave function, usually determined by means of variational calculations, and \(G_0\) is an approximation to the Green’s function of the imaginary time Schrödinger equation:

\[
G_0(X, X', t) = \left(4\pi Dt\right)^{-3A/2}e^{-(R-R')^2/4Dt}e^{-t(V(X)-E_0)}, \tag{2}
\]

where \(D = \hbar^2/2m\), \(E_0\) is an estimate of the ground state energy of the system, and \(V(X)\) is the nucleon–nucleon interaction. For a long enough imaginary time the distribution of the walkers converges to the product \(\Psi_T(X)\Psi_0(X)\) where \(\Psi_0\) is the wave function of the ground state of \(H\). This fact allows the computation of matrix elements \(\langle \Psi_T|\hat{O}|\Psi_0\rangle\) of observables \(\hat{O}\) of interest in a Monte Carlo way. When \(\hat{O} \equiv \hat{H}\) the value obtained is the exact ground state energy of the system.

The presence of an interaction \(V(X)\) including operators like \((3\vec{\sigma}_i \cdot \vec{r}_{ij} \vec{\sigma}_j\cdot \vec{r}_{ij} - \vec{\sigma}_i \cdot \vec{\sigma}_j)\) and \(\vec{\tau}_i \cdot \vec{\tau}_j\) is the origin of the computational cost in the standard approaches. AFDMC uses the Hubbard–Stratonovich method to transform the operators \(\hat{S}\) which are quadratic in the spin and isospin into linear operators:

\[
e^{-(1/2)\lambda \hat{S}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dy e^{-y^2/2} e^{y\sqrt{-\lambda} \hat{S}} \tag{3}
\]

Then \(\hat{S}\) are operators which are linear combinations of the spin and isospin operators for each nucleon, and \(\lambda\) depend on the interaction. The transformed Green’s Function is applied to the spin-isospin part of the wave function, and its effect consists of a rotation of the spin and isospin degrees of freedom (written as four-component spinors in the proton-neutron up-down basis) by a quantity that depends on the auxiliary variable \(y\) along
with multiplication of the state by an overall factor. The sum over spin and isospin is replaced by sampling a set of rotations of the variables. This procedure reduces the dependence of the computational time on the number of nucleons necessary for performing a simulation step from exponential to cubic. It is therefore possible to perform on a regular workstation or on a modest PC cluster calculations that would require Ttlop supercomputers with the standard methods. This method, like other diffusion Monte Carlo methods, suffers from the so-called “sign problem” when it is applied to fermions, and when complex wave functions need to be used. In our calculations we apply the fixed-phase approximation to overcome this problem.\(^\text{18}\)

While this method has already been successfully applied to pure neutron matter,\(^\text{15}\) it has not been previously used for mixed proton and neutron systems. It should be noted that it does not guarantee an upper bound to the mixed energy used here. As a test for the correctness and the efficiency of our approach we reproduced within 0.3 MeV total energy the existing results for the binding energy of \(^4\text{He}\) with potentials of the AV6 class.\(^\text{19}\) We have also been able to compute binding energies for \(^{16}\text{O}\) and for \(^{40}\text{Ca}\) with this method.

### 3. INTERACTION

A crucial point in dealing with nuclear matter is the choice of the interaction among nucleons. As already mentioned, several modern two–body potentials are available nowadays, all fitting the NN data with \(\chi^2 \sim 1\). We use the potentials of the Argonne class with \(n\) operators (AV\(n\)).\(^\text{21}\) While the full version contains \(n = 18\) operators, most of the physics is reasonably well described by the first 6 operators made up of 4 central spin–isospin dependent components and two tensor ones, which include the long range one–pion–exchange force. The most important missing terms are the spin–orbit components. In nuclei and neutron drops the spin–orbit contribution to the energy amounts to a few tenths of MeV/nucleon. A correction of the order 1MeV/nucleon can be attributed at low densities to the remaining terms included in AV18. Specifically, we have used the interaction Argonne \(v'_{s}\)\(^\text{19}\) truncated by dropping the spin–orbit terms, and including only the first six operators, which we denote as AV6'.

It is well known that two–body NN interaction underbind light nuclei, and one needs to add a specific effective three–body potential to reproduce their low energy properties. Semi–phenomenological three–nucleon interactions following the lowest order three–nucleon diagrams with one and two intermediate Delta resonance states provide a very satisfactory description
of the ground state energy and the low level spectra of light nuclei up to $^{12}$C. We have disregarded such three-body forces in our simulations. In nuclear matter they are essential to reproduce the experimental saturation density, and, in general, they contribute about 10% of the total binding energy. A full comparison with the available experimental data goes beyond the scopes of the present paper. Here we are interested in showing the efficiency of the AFDMC methods in dealing with nuclear matter models which include realistic tensor interactions like in the AV6’ potential.

4. RESULTS

The results of the calculations with $A=28$ include box corrections that have computed by adding to the two body sums contribution of nucleons in the first shell of periodic cells. Such procedure is effective. In order to assess the magnitude of finite size effects we performed calculations with 76 and 108 nucleons at densities $\rho = 0.08\ \text{fm}^{-3}$ and $\rho = 0.48\ \text{fm}^{-3}$. The results coincide with the ones obtained with 28 nucleons within 3 percent.

We computed the EOS of symmetric nuclear matter in the range of densities $0.5 \leq (\rho/\rho_0) \leq 3$, and compared it with previous available results obtained with the same potential using Fermi Hypernetted Chain in the Single Operator Chain approximation (FHNC/SOC) and the Brueckner-Hartree-Fock (BHF) in the two–hole line approximation. AFDMC calculations were performed with 28 nucleons, filling the shell of plane waves with momentum of modulus 1 and providing a wave function yielding an isotropic density.

The results are summarized in Fig. 1 and reported in Ref. 12. The comparison of the various EOS suggests the following comments: FHNC/SOC leads to an overbinding at high density. A similar indication was found by Moroni et al. after a DMC calculation of the EOS of normal liquid $^3$He at zero temperature, with a guiding function including triplet and backflow correlations. The comparison with the equivalent FHNC/SOC calculations of Refs. 24,25 have shown similar discrepancies. There are two main intrinsic approximations in variational FHNC/SOC calculations, which violate the variational principle. The first one consists in neglecting a whole class of cluster diagrams, the so called elementary diagrams, which cannot be summed up by means of FHNC integral equations. We have calculated the lowest order diagram of this class, namely the one having only one correlation bond and four exchange bonds. The results obtained show a substantial effect from this diagram and bring the FHNC/SOC estimates very close to AFDMC results, as shown in Fig. 1. The second approximation is related
to the non-commutativity of the correlation operators entering the variational wave function. The only class of cluster diagrams contributing to such non-commuting terms, which can be realistically calculated, is that characterized by single operator chains. It is believed that such an approximation is reliable in nuclear matter, but there is no clear proof of this.

BHF calculations of ref.\textsuperscript{22} predict an EOS with a shallower binding than the AFDMC one. It has been shown for symmetric nuclear matter, using the AV18 and AV14 potentials, that contributions from three hole–line diagrams add a repulsive contribution up to $\sim 3\text{MeV}$ at densities below $\rho_0$,\textsuperscript{26} and decrease the energy at high densities.\textsuperscript{27} Such corrections, if computed with the AV6$'$ potential, would probably preserve the same general behavior, and bring the BHF EOS closer to the AFDMC one. Therefore, our calculations show that the two hole–line approximation used in Ref. 22 is too poor, particularly at high density.

The AFDMC equation of state was fitted with the following functional form:

$$
\frac{E}{A} = \frac{E_0}{A} + \alpha(x - \bar{x})^2 + \beta(x - \bar{x})^3, \quad (4)
$$
where $x = \rho/\rho_0$ and the various coefficients are given by $E_0/A = -14.04(4)$ MeV, $\alpha = 3.09(6)$ MeV, $\beta = -0.44(8)$ MeV, and $\bar{x} = 1.83(1)$. The resulting compressibility $K = 9\bar{x}^2 \left( \frac{\partial^2 (E/A)}{\partial x^2} \right) \bar{x}$ at saturation density $\bar{x}$ is $\sim 190$ MeV. The fit of the EOS allows for computing the pressure vs. density for symmetric nuclear matter.

5. CONCLUSIONS

The availability of an efficient and relatively fast projection algorithm for the computation of energies and other observables of dense hadronic matter enables the possibility of a more quantitative understanding of the properties of neutron stars and supernovae, as well as that of medium–heavy nuclei. Computations on such systems are at present out of reach of the standard GFMC methods and available supercomputers. Therefore, the extension of AFDMC algorithm to deal with nuclear matter is a significant step forward. Some technical improvements on the calculations presented here, such as the addition to the AV6’ of spin–orbit terms and three–body interactions are already underway. The treatment of asymmetric nuclear matter, particularly important for the determination of the properties of neutron stars, is also straightforward, and will be the subject of future exploration.

We acknowledge helpful conversations with M.H. Kalos, P. Faccioli, W. Leidemann, E. Lipparini, and G. Orlandini. This work was in part supported by NSF grant PHY-0456609. Calculations were performed on the HPC facility "BEN" at ECT* in Trento under a grant for Supercomputing Projects.

References

1. J. Piekarewicz, Phys. Rev. C 69, p. 041301 (2004).
2. J. Morales, Jr., V. R. Pandharipande and D. G. Ravenhall, Phys. Rev. C 66, p. 054308 (2002).
3. A. Akmal, V. R. Pandharipande and D. G. Ravenhall, Phys. Rev. C 58, p. 1804 (1998).
4. V. R. Pandharipande and R. B. Wiringa, Rev. Mod. Phys. 51, p. 821 (1979).
5. H. Kamada, A. Nogga, W. Glockle, E. Hiyama, M. Kamimura, K. Varga, Y. Suzuki, M. Viviani, A. Kievska, S. Rosati, J. Carlson, S. C. Pieper, R. B. Wiringa, P. Návratil, B. R. Barrett, N. Barnea, W. Leidemann and G. Orlandini, Phys. Rev. C 64, p. 044001 (2001).
6. D. Gutz, S. Bacca, N. Barnea, W. Leidemann and G. Orlandini, Phys. Rev. Lett. 96, p. 112301 (2006).
7. J. Carlson and R. Schiavilla, Rev. Mod. Phys. 70, p. 743 (1998).
8. P. Navrátil, J. P. Vary and B. R. Barrett, *Phys. Rev. Lett.* **84**, p. 5728 (2000).
9. S. C. Pieper, *Nucl. Phys. A* **751**, p. 516 (2005).
10. S. C. Pieper, K. Varga and R. B. Wiringa, *Phys. Rev. C* **66**, p. 044310 (2002).
11. J. Carlson, J. Morales, Jr., V. R. Pandharipande and D. G. Ravenhall, *Phys. Rev. C* **68**, p. 025802 (2003).
12. S. Gandolfi, F. Pederiva, S. Fantoni and K. E. Schmidt, *nucl-th/0607022*.
13. K. E. Schmidt and S. Fantoni, *Phys. Lett. B* **446**, p. 99 (1999).
14. S. Fantoni, A. Sarsa and K. E. Schmidt, *Phys. Rev. Lett.* **87**, p. 181101 (2001).
15. A. Sarsa, S. Fantoni, K. E. Schmidt and F. Pederiva, *Phys. Rev. C* **68**, p. 024308 (2003).
16. S. Gandolfi, F. Pederiva, S. Fantoni and K. E. Schmidt, *Phys. Rev. C* **73**, p. 044304 (2006).
17. F. Pederiva, A. Sarsa, K. E. Schmidt and S. Fantoni, *Nucl. Phys. A* **742**, p. 255 (2004).
18. S. Zhang and H. Krakauer, *Phys. Rev. Lett.* **90**, p. 136401 (2003).
19. R. B. Wiringa and S. C. Pieper, *Phys. Rev. Lett.* **89**, p. 182501 (2002).
20. S. Gandolfi, F. Pederiva, S. Fantoni and K. E. Schmidt, *in preparation*.
21. R. B. Wiringa, V. G. J. Stoks and R. Schiavilla, *Phys. Rev. C* **51**, p. 38 (1995).
22. I. Bombaci, A. Fabrocini, A. Polls and I. Vidaña, *Phys. Lett. B* **609**, p. 232 (2005).
23. S. Moroni, S. Fantoni and G. Senatore, *Phys. Rev. B* **52**, p. 13547 (1995).
24. E. Manousakis, S. Fantoni, V. R. Pandharipande and Q. N. Usmani, *Phys. Rev. B* **28**, p. 3770 (1983).
25. M. Viviani, E. Buendia, S. Fantoni and S. Rosati, *Phys. Rev. B* **38**, p. 4523 (1988).
26. H. Q. Song, M. Baldo, G. Giansiracusa and U. Lombardo, *Phys. Rev. Lett.* **81**, p. 1584 (1998).
27. M. Baldo, A. Fiasconaro, H. Q. Song, G. Giansiracusa and U. Lombardo, *Phys. Rev. C* **65**, p. 017303 (2001).