Monte Carlo approach to nuclei and nuclear matter

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Abstract. We report on the most recent applications of the Auxiliary Field Diffusion Monte Carlo (AFDMC) method. The equation of state (EOS) for pure neutron matter in both normal and BCS phase and the superfluid gap in the low–density regime are computed, using a realistic Hamiltonian containing the Argonne AV8’ plus Urbana IX three–nucleon interaction. Preliminary results for the EOS of isospin–asymmetric nuclear matter are also presented.

Keywords: nuclear matter, asymmetric nuclear matter, neutron matter, equation of state, nuclei, superfluid gap, Quantum Monte Carlo
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INTRODUCTION

The improved accuracy of experimental data on nuclei, together with a rediscovered role of nuclear matter properties in the understanding of nuclear structure and several phenomena of astrophysical interest[1], has shown the need for a more detailed investigation of the ground state of nuclear many–body systems.

Recent realistic nuclear Hamiltonians have been used to compute properties of light nuclei in very good agreement with experiments[2]. However, the physical properties of nuclear and neutron matter could be very different from that of nuclei; in fact the nucleon density in the core of heavy nuclei reaches the maximum value of $\rho_0=0.16$ fm$^{-1}$, while the relevant range of density of matter inside neutron stars is up to 9 times $\rho_0$[3]. Therefore we are now facing, on one side, the problem of finding a fundamental scheme for the description of nuclear forces, valid from the deuteron up to dense nuclear matter, which is still an open fundamental problem, and, on the other, that of solving a many–body problem which is made extremely complex by the strong spin–isospin dependence of the forces. In this paper we will not address the problem of determining the nuclear force. We will consider a nuclear Hamiltonian which provides good fits to the N–N data up to meson production and reproduces fairly well the ground state and the low energy spectra of light nuclei. This is made of two– and three-body spin–isospin dependent potential. We present results for the ground state of large nuclear systems with this Hamiltonian.

It is well known that Quantum Monte Carlo (QMC) methods can provide estimates
of physical observables at the best known accuracy\cite{4}, and they are therefore useful to
gauge the validity of proposed interaction models without having the bias of using more
approximate methods.

A new generation of powerful QMC techniques have been recently devised to simu-
late large nucleonic systems with up to hundred of nucleons: the Auxiliary Field Diffu-
sion Monte Carlo (AFDMC)\cite{5}. They have been used to compute the EOS of nuclear
matter\cite{6}, showing important limitations of other many–body methods and of the mod-
ern nuclear interactions based on two– plus three–body potentials in the high density
regime. The accuracy of AFDMC was demonstrated by comparing the ground state of
light nuclei with results provided by Green’s Function Monte Carlo (GFMC)\cite{7} that is
known to give accurate results for the properties of light nuclei up to A=12\cite{2}. By sam-
pling the spin–isospin states of the nucleons AFDMC can be applied to large systems;
it was used to simulate the ground state of medium sized nuclei up to A=40\cite{8}, nu-
clear matter with up to A=108\cite{6}, the properties of neutron–rich nuclei\cite{9,10}, neutron
drops\cite{11}, and neutron matter with up to A=114\cite{11,12,13}.

In this paper we discuss the latest results of the computation of the equation of state
(EOS) of neutron matter in both the normal and superfluid phases, the computation of
the superfluid gap of neutron matter in the low–density regime, and some preliminary
results about the EOS of isospin-asymmetric nuclear matter.

**HAMILTONIAN**

The ground state of nuclear systems can be realistically studied by starting from the
non–relativistic nuclear Hamiltonian of the form

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

(1)

where $m$ is the averaged mass of proton and neutron, and $v_{ij}$ and $V_{ijk}$ are two– and
three–body potentials; it seems that the effect of forces due to $n$–body terms with
$n > 3$ in the low energy properties of light nuclei is negligible. Such a form for the
Hamiltonian has been shown to describe properties of light nuclei in excellent agreement
with experimental data (see Ref. \cite{2} and references therein). All the degrees of freedom
responsible for the interaction between nucleons (such the $\pi$, $\rho$, $\Delta$, etc.) are integrated
out and included in $v_{ij}$ and $V_{ijk}$.

At present, several realistic nucleon–nucleon interactions (NN) fit scattering data with
very high precision. We consider the NN potentials belonging to the Argonne family.
Such interactions are written as a sum of operators:

$$v_{ij} = \sum_{p=1}^{M} v_p(r_{ij}) O^{(p)}(i,j),$$

(2)

where $O^{(p)}(i,j)$ are spin–isospin dependent operators. The number of operators $M$
characterizes the interaction; the most accurate of them is the Argonne AV18 with
$M=18$\cite{14}. Here we consider some simpler forms derived from AV18, namely the AV8’
and the AV6'\cite{15} with a smaller number of operators. For many systems, the difference between these simpler forms and the full AV18 potential can be computed perturbatively. Most of the contribution of the NN is due to the one pion exchange between nucleons, but the effect of other mesons exchange as well as some phenomenological terms are included.

The eight $O^{(p)}(i,j)$ terms in AV8' are given by the four central components $1$, $\vec{\tau}_i \cdot \vec{\tau}_j$, $\vec{\sigma}_i \cdot \vec{\sigma}_j$, $(\vec{\sigma}_i \cdot \vec{\sigma}_j)(\vec{\tau}_i \cdot \vec{\tau}_j)$, the tensor $S_{ij}$, the tensor–$\tau$ component $S_{ij} \vec{\tau}_i \cdot \vec{\tau}_j$, where $S_{ij} = 3(\vec{\sigma}_i \cdot \vec{\tau}_j)(\vec{\sigma}_j \cdot \vec{\tau}_j) - \vec{\sigma}_i \cdot \vec{\sigma}_j$, the spin–orbit $\vec{L}_{ij} \cdot \vec{\tau}_{ij}$ and the spin–orbit–$\tau$ $(\vec{L}_{ij} \cdot \vec{S}_{ij})(\vec{\tau}_i \cdot \vec{\tau}_j)$, where $\vec{L}_{ij}$ and $\vec{S}_{ij}$ are the total angular momentum and the total spin of the pair $ij$.

The AV6' has the same structure of AV8', but the spin–orbit operators are dropped. In general, all the AVx' interactions are obtained starting from the AV18, written by dropping less important operators, and refitted in order to keep the most important features of NN in the scattering data\cite{15}.

The three–body interactions (TNI) is essential to overcome the underbinding of nuclei with more than two nucleons. The NN is fitted to scattering data and correctly gives the deuteron binding energy, but starting with $^3H$ the NN is not sufficient to describe the ground state of light nuclei. The Urbana-IX (UIX) potential corrects this limitation of NN, and was fitted to light nuclei and to correctly reproduce the expected saturation energy of nuclear matter\cite{16}. It essentially contains the Fujita–Miyazawa term\cite{17} that describes the exchange of two pions between three nucleons, with the creation of an intermediate excited $\Delta$ state. Again, a phenomenological part is required to sum all the other neglected terms. The generic form of UIX is the following:

$$V_{ijk} = V_{2\pi} + V_R.$$ (3)

The Fujita-Miyazawa term\cite{17} is spin–isospin dependent:

$$V_{2\pi} = A_{2\pi} \sum_{\text{cyc}} \left[ X_{ij}, X_{jk} \right] \left\{ \tau_i \cdot \tau_j, \tau_j \cdot \tau_k \right\} + \frac{1}{4} \left[ X_{ij}, X_{jk} \right] \left[ \tau_i \cdot \tau_j, \tau_j \cdot \tau_k \right],$$ (4)

where the $X_{ij}$ operators describe the one pion exchange, and their structure is the same of that of AV6'. The phenomenological part is

$$V_{R} = U_0 \sum_{\text{cyc}} T^2(m_{\pi} r_{ij}) T^2(m_{\pi} r_{jk}).$$ (5)

The factors $A_{2\pi}$ and $U_0$ are kept as fitting parameters. The binding energy of symmetrical nuclear matter is not well reproduced by such force. Other forms of TNI, called Illinois forces\cite{18}, which includes three–nucleon Feynman diagrams with two Deltas intermediate states, are available. However, they provide unrealistic overbinding of neutron systems when density increases\cite{11,12} and they do not seem to describe realistically high density (already at $\rho \geq \rho_0$) nucleonic systems.

**THE AFDMC METHOD**

Ground state AFDMC simulations rely, as do other traditional QMC methods, on previous variational calculations, often performed within FHNC theory\cite{19}, to compute a
trial wave function $\Psi_T$, which is used to guide the sampling of the random walk. A typical form for $\Psi_T$ is given by a correlation operator $\hat{F}$ operating on a mean field wave function $\Phi(R)$,

$$\langle R, S | \Psi_T \rangle = \hat{F} \Phi(R).$$

Mean field wave functions $\Phi(R)$ that have been used are: (i) a Slater determinant $\Phi_{FG}$ of plane wave orbitals for nuclear and neutron matter in the normal phase, (ii) a linear combination $\Phi_{sp}$ of a small number of antisymmetric products of single particle orbitals $\phi_j(\vec{r}_i, s_i)$ for nuclei and neutron drops, and (iii) a pfaffian $\Phi_{pf}$, namely an antisymmetric product of independent pairs for neutron matter in superfluid phase.

A realistic correlation operator is the one provided by FHNC/SOC theory, namely

$$\mathcal{S} \prod_{j>i} f^{(p)}(r_{ij}) O^{(p)}(i,j),$$

where $\mathcal{S}$ is the symmetrizer and the operators $O^{(p)}(i,j)$ are the same as those appearing in the two–body potential.

Unfortunately, the evaluation of this wave function requires exponentially increasing computational time with the number of particles. This procedure is followed in variational and Green’s function Monte Carlo calculations, where the full sum over spin and isospin degrees of freedom is carried out. Since for large numbers of particles it is not computationally feasible to evaluate these trial functions, the much simpler correlation operator $\prod_{j>i} f^{c}(r_{ij})$, which contains the central Jastrow correlation only, is used instead. The evaluation of the corresponding trial function requires order $A^3$ operations to evaluate the Slater determinants and $A^2$ operations for the central Jastrow. Since many important correlations are neglected in these simplified functions, we use the Hamiltonian itself to define the spin sampling.

The AFDMC method works much like Diffusion Monte Carlo[4, 5, 20, 21, 9]. The wave function is defined by a set of what we call walkers. Each walker is a set of the 3A coordinates of the particles plus a number $A$ of four component spinors each representing a spin–isospin state. The imaginary time propagator for the kinetic energy and the spin–independent part of the potential is identical to that used in standard diffusion Monte Carlo. The new positions are sampled from a drifted Gaussian with a weight factor for branching given by the local energy of these components. Since they do not change the spin state, the spinors will be unchanged by these parts of the propagator.

To sample the spinors we first use a Hubbard Stratonovich transformation to write the propagator as an integral over auxiliary fields of a separated product of single particle spin–isospin operators. We then sample the auxiliary field value, and the resulting sample independently changes each spinor for each particle in the sample, giving a new sampled walker.

More details about the AFDMC method can be found in Ref. [11].

**NUCLEONIC MATTER**

The properties of nuclear matter, like the Equation of State (EOS), are of fundamental importance in nuclear physics, mainly because nuclei behave very much like liquid drops. Indeed, each of these can be associated with a mass formula, which fits the corresponding data of stable nuclei from $A \sim 20$ on. Any such mass formula has a
volume and a symmetry term provided by symmetrical nuclear matter and nuclear matter with $N > Z$ respectively. Moreover, accurate model independent calculations of the above observables are much needed in the physics of heavy ion reactions, as well as in that of lepton and neutrino scattering off nuclei at intermediate energies. Medium effects have to be taken into account for the data analysis of such reactions at the present level of accuracy.

In addition, the theoretical knowledge of the properties of asymmetric nuclear matter at low temperature is needed to predict the structure, the dynamics and the evolution of stars, in particular during their last stages, when they become ultra–dense neutron stars.

We present in the following the results obtained with AFDMC for the EOS of pure neutron matter in normal phase, as well as the gap of the BCS phase of neutron matter\cite{11, 22, 13}. Previously results of the EOS of nuclear matter and nuclei can be found in Refs. \cite{6, 8, 11}.

Neutron matter is simulated by considering $N$ neutrons in a periodic box, and particular care is taken to evaluate the effects due to the finite size of the box. More details can be found in Refs. \cite{12, 11}.

In Fig. 1 we plot the AFDMC equation of state, obtained with the energy of 66 neutrons, and the variational calculation of Akmal et al. of Ref. \cite{23}, where the AV18 NN interaction combined with the Urbana UIX TNI was considered. As it can be seen both the AV8' and the AV18 essentially give an EOS with the same behavior, but the addition of the TNI adds some differences, in particular at higher densities.

The AV8' interaction should be more attractive than AV18 as shown in light nuclei and in neutron drop calculation\cite{7}. This result is not confirmed by our calculations as it is clearly visible in Fig. 1. The AFDMC has proved to be in very good agreement with the GFMC results for light nuclei\cite{8}, and we believe that the same accuracy is reached in the neutron matter calculation, as shown in the comparison with the GFMC results of 14 neutrons\cite{11, 13}. On the other hand the AFDMC calculation of the nuclear matter have shown that FHNC/SOC does not seem to provide safe energy upperbounds. This is because of the lack of cluster diagrams with commutator terms beyond the SOC approximation and that of elementary diagrams, not included in the FHNC summation\cite{6}.
FIGURE 2. The EOS of neutron matter in the low–density regime. The two calculations were performed using different trial wave functions modeling a normal and a BCS state.

The addition of the UIX three–body interaction to the Hamiltonian increases the differences between the AFDMC results and that of Akmal et al. The difference cannot be due to finite–size effects in our calculation for the following reason: the total contribution of UIX should be positive in neutron matter, so that the inclusion of box corrections as done for the two–body part of the Hamiltonian would eventually increase the total energy. The periodic box–FHNC estimation of these effect essentially confirms this observation[12].

It is worth observing how important the three–nucleon interaction already is at medium–high densities. Its contribution at $2\rho_0$ is $\sim 25$MeV and increases very rapidly with density. The four Illinois potentials[18], built to include two $\Delta$ intermediate states in the three nucleon processes, lead to very different results compared to the Urbana IX[12,11] EOS at medium–high densities, in spite of the fact that all of them provide a satisfactory fit to the ground state and the low energy spectrum of nuclei with $A \leq 8$. This, once more, points outs the importance of understanding the role of $n$–body forces with $n > 3$ in nuclear astrophysics.

We explored the superfluid phase of low–density neutron matter. Because the AFDMC projects out the lowest energy state with the same symmetry and phase as the trial wave function, we tried to repeat some calculation using a BCS trial wave function of the form of Ref. [24]. The BCS state provides an energy that is lower than the normal state, however the difference never exceeds 3% of the total energy. We report the energy per neutron in the low–density regime evaluated using a normal and a BCS trial wave function in Fig. 2.

In the low–density regime the neutron matter is in a $^1S_0$ superfluid phase. In this regime, the neutron–neutron interaction is dominated by this channel, whose scattering length is very large and negative, about $a=-18.5$ fm. Several attempts to compute the pairing gap using a bare effective interaction like those used for cold atom problems have been performed in the last few years[22]. However, our results show that an accurate calculation of the superfluid gap in this regime must include the full Hamiltonian instead of one describing the $^1S_0$ physics only.

We computed the superfluid gap by means of AFDMC that allows for quantum simulations of the superfluid phase of neutron matter, by solving the ground state of
FIGURE 3. The superfluid gap computed using AFDMC and compared with other techniques is displayed.

FIGURE 4. The EOS of nuclear matter as a function of the density and of the isospin–asymmetry. See the text for details.

the full Hamiltonian with AV8’+UIX without the use of some simplified interaction. In Fig. 3 the AFDMC gap is compared with standard BCS theory and some other often referred calculations based upon to correlated theories at two–body approximation (see also Ref. [13]).

The computation of the isospin–asymmetric nuclear matter is possible with a trivial modification of the trial wave function used to project out the ground state of the system. The asymmetry is defined by

$$\alpha = \frac{N - Z}{N + Z},$$

(7)

where $N$ is the number of neutrons and $Z$ of protons. We report in Fig. 4 preliminary results of the EOS of nuclear matter for different values of $\alpha$, using a simplified Hamiltonian containing the AV6’ NN interaction. The various curves of the figure from the top to the bottom are in the same order of the legend, where it is also indicated the number of neutrons and protons for each simulation.

As displayed in the legend of Fig. 4 some calculations were performed using a very small number of protons. These results could suffer important finite size effects. The
study of finite size effect particularly due to the kinetic energy is in progress. It is possible to reduce the dependence of the kinetic energy on the number of particles by using different kinds of periodic boundary conditions: e.g. the so called twist average boundary conditions (TABC) [25]. The computation of several EOS by using TABC to see the effect to the kinetic energy is in progress.

CONCLUSIONS AND PERSPECTIVES

We have briefly shown some recent results obtained using AFDMC theory. This recently developed Quantum Monte Carlo provides results for the binding energy of light nuclei [8] and neutron drops [11] which are is very good agreement with accurate GFMC calculations. However, unlike those methods AFDMC is well suited to deal with nucleonic systems with up to hundred of nucleons in the Hamiltonian.

We have presented AFDMC results for the EOS of neutron matter in the normal phase [13]. In the low–density regime where neutrons form a superfluid phase, we modified the trial wave function in order to include important BCS correlations to compute the superfluid gap of neutron matter [22]. Preliminary results for the EOS of asymmetric nuclear matter have also been presented and discussed.

It should be stressed that, besides having shown that AFDMC theory opens up the possibility of studying the properties of large nucleonic systems, with an accuracy which goes much beyond that of other commonly used many–body theories, the results we have already obtained indicate serious inadequacies of commonly used nuclear interactions in the high density regime, of interest in astronuclear physics.

The problem of determining the nuclear Hamiltonian, and in particular the effect of \( n \)–body forces with \( n > 3 \) is becoming of primarily importance. We are working on developing a new form for the interaction that perturbatively contains the excitation of nucleons. The corresponding potential naturally generates many-body forces, that should be small in nuclei, but of primary importance in nuclear and neutron matter.

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