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A quantum Monte Carlo method for nucleon systems

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Abstract

We describe a quantum Monte Carlo method for Hamiltonians which include tensor and other spin interactions such as those that are commonly encountered in nuclear structure calculations. The main ingredients are a Hubbard-Stratonovich transformation to uncouple the spin degrees of freedom along with a fixed node approximation to maintain stability. We apply the method to neutron matter interacting with a central, spin-exchange, and tensor forces. The addition of isospin degrees of freedom is straightforward.

1. Introduction

Much of nuclear physics can be described by a model of mesons and nucleons. For many problems in nuclear structure the mesons are integrated out to produce a nuclear Hamiltonian which has different interactions in different angular momentum channels. Simplified interactions that have most of the main features of the nucleon-nucleon interaction are given by potential models such as the Urbana v_{14} [1] or Argonne v_{18} [2] potentials. These potentials have the form

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

where i and j label the two nucleons, r_{ij} is the distance separating the two nucleons, and the $O^{(p)}$ include spin, isospin, and spin orbit operators, and M is the maximum number of operators (i.e. 14 in v_{14} models).

The inclusion of the spin and isospin operators makes standard quantum Monte Carlo methods much more difficult. The number of spin-isospin states for a nucleus with Z protons and A nucleons is

$$\frac{A!}{Z!(A-Z)!} 2^A \tag{2}$$

which quickly becomes intractable as A gets large. Green's function Monte Carlo methods that include all the spin-isospin states have been carried out only for light nuclei ($A \lesssim 8$) [3].

Nuclear quantum Monte Carlo not only has a continuum of spatial positions, but also has a ''lattice'' of spin configurations with nonlocal propagators. A similar situation occurs in quantum Monte Carlo calculations with explicit lattice Hamiltonians. Recently, constrained path quantum Monte Carlo methods have given good results for these lattice systems [4,5]. Our method is to apply these same

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constrained path techniques for the spin lattice to both deal with the large number of spin degrees of freedom and to stabilize the algorithm so that the well known fermion sign problem can be controlled [6]. The spatial part of the Hamiltonian is done with standard Green's function or diffusion Monte Carlo [7,8]. For the case where the interaction is spin and isospin independent, our method reduces to the standard fixed node method [8,9].

2. The method for the v_6 potential

While we believe that our method can be applied at least approximately to spin orbit interactions, we have not verified this in detail, and in this paper we will talk specifically about spin-isospin dependent interactions that are present in v_6 models. Since these models include the full spin-isospin problem of the more detailed models, this truncation is not a fundamental limitation, and the v_6 models contain most of the physics of the nucleon-nucleon interaction. These potentials are given by Eq. (1) with the operators, $O^n(i,j)$; 1 is the central operator, and the spin isospin operators $\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$, $\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$, t_{ij}, and $t_{ij}\boldsymbol{\tau}\cdot\boldsymbol{\tau}_j$, where t_{ij} is the tensor operator $3\boldsymbol{\sigma}_i\cdot\hat{r}_{ij}\boldsymbol{\sigma}_j\cdot\hat{r}_{ij}-\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j$. The $\boldsymbol{\tau}_i$ and $\boldsymbol{\sigma}_i$ are the Pauli matrices for the isospin and spin of particle i.

For N particles, the v_6 interaction can be written as

$$\begin{aligned}V&=\sum_{i<j}\left[\sum_{p=1}^{6}v_p(r_{ij})O^{(p)}(i,j)\right]\\&=V_{\rm c}+V_{\rm nc}\\&=V_{\rm c}+\frac{1}{2}\sum_{i,\alpha,j,\beta}\sigma_{i,\alpha}A^{(\sigma)}_{i,\alpha,j,\beta}\sigma_{j,\beta}\\&\quad+\frac{1}{2}\sum_{i,\alpha,j,\beta}\sigma_{i,\alpha}A^{(\sigma\tau)}_{i,\alpha,j,\beta}\sigma_{j,\beta}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\\&\quad+\frac{1}{2}\sum_{i,j}A^{(\tau)}_{i,j}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\end{aligned}\tag{3}$$

where $V_{\rm c}$ is the sum of the central interactions

$$V_{\rm c}=\sum_{i<j}v_1(r_{ij}),\tag{4}$$

and the noncentral potential $V_{\rm nc}$ contains the operator dependence. The roman indices, i, j, etc. indicate particle number and the greek indices the cartesian component of the operators. In our example calculations we deal only with neutron matter. In this case, the $\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j$ isospin operator evaluates to 1, the $v^{(2)}$ term is included in $V_{\rm c}$ and only the A^{σ} term is needed to give the noncentral interactions.

We define the A matrices in Eq. (3) so that they are zero when $i=j$ and take them to be symmetric. While many other choices are possible, with this choice, all the A matrices are real and symmetric and have real eigenvalues and eigenvectors. We define these eigenvectors and eigenvalues as

$$\sum_{j,\beta}A^{(\sigma)}_{i,\alpha,j,\beta}\boldsymbol{\psi}^{\sigma}_n(j)\cdot\hat{x}_\beta=\lambda^{(\sigma)}_n\boldsymbol{\psi}^{\sigma}_n(i)\cdot\hat{x}_\alpha\tag{5}$$

and similarly for the $\sigma\tau$ and τ cases.

The matrices can be written in terms of their eigenvectors and eigenvalues to give the noncentral potential

$$\begin{aligned}V_{\rm nc}&=\frac{1}{2}\sum_{i,j,n}\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\sigma)}_n(i)\lambda^{(\sigma)}_n\boldsymbol{\psi}^{(\sigma)}_n(j)\cdot\boldsymbol{\sigma}_j\\&\quad+\frac{1}{2}\sum_{i,j,n}\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\sigma\tau)}_n(i)\lambda^{(\sigma\tau)}_n\boldsymbol{\psi}^{(\sigma\tau)}_n(j)\cdot\boldsymbol{\sigma}_j\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\\&\quad+\frac{1}{2}\sum_{i,j,n}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\psi^{(\tau)}_n(i)\lambda^{(\tau)}_n\psi^{(\tau)}_n(j)\end{aligned}\tag{6}$$

These can be rewritten as

$$\begin{aligned}V_{\rm nc}&=\frac{1}{2}\sum_{n=1}^{3N}\left(O^{(\sigma)}_n\right)^2\lambda^{(\sigma)}_n\\&\quad+\frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{3N}\left(O^{(\sigma\tau)}_{n\alpha}\right)^2\lambda^{(\sigma\tau)}_n\\&\quad+\frac{1}{2}\sum_{\alpha=1}^{3}\sum_{n=1}^{N}\left(O^{(\tau)}_{n\alpha}\right)^2\lambda^{(\tau)}_n\end{aligned}\tag{7}$$

with

$$\begin{aligned}O^{(\sigma)}_n&=\sum_i\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\tau)}_n(i),\\O^{(\sigma\tau)}_{n\alpha}&=\sum_i\tau_{i\alpha}\boldsymbol{\sigma}_i\cdot\boldsymbol{\psi}^{(\sigma\tau)}_n(i),\\O^{(\tau)}_{n\alpha}&=\sum_i\tau_{i\alpha}\psi^{(\tau)}_n(i)\end{aligned}\tag{8}$$

We can now use the Hubbard-Stratonovich method to write the exponential of the potential multiplied by the time step that is needed in Green's function or diffusion Monte Carlo [10]. The Hubbard-Stratonovich transformation is given by the Gaussian integration,

$$e^{-\frac{1}{2}\lambda_n O_n^2\,\Delta t} = \left(\frac{\Delta t|\lambda_n|}{2\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}\Delta t|\lambda_n|x^2 - \Delta t s \lambda_n O_n x} \tag{9}$$

where s is 1 for $\lambda < 0$, and s is i for $\lambda > 0$.

Our O_n don't commute, so we need to keep the time steps small so that the commutator terms can be ignored. Each of the O_n is a sum of 1-body operators, so we can easily operate them on our spin states.

A discrete version of this transformation is given by Koonin et al. [11]. It is essentially a three point Simpson's rule integration of the gaussian centered on the origin with the step size selected to optimize the order. Modified for our notation, it is

$$e^{-\frac{1}{2}\lambda_n O_n^2\,\Delta t} = \int_{-\infty}^{\infty} dx f(x)\, e^{-\Delta t s \lambda_n O_n x} + \mathrm{Order}(\Delta t^3), \tag{10}$$

where

$$f(x) = \tfrac{1}{6}\left[\delta(x-h) + 4\delta(x) + \delta(x+h)\right],$$

$$h = \left(\frac{3}{|\lambda_n|\Delta t}\right)^{\frac{1}{2}}. \tag{11}$$

We require $3N$ Hubbard-Stratonovich variables for the σ terms, $9N$ variables for the $\sigma\tau$ terms, and $3N$ variables for the τ terms. Each time step requires the diagonalization of two $3N$ by $3N$ matrices and one N by N matrix. Many other breakups are possible. We could, for example, break up each pair potential exactly as above, we would not need the matrix diagonalizations, but we would require more Hubbard-Stratonovich variables. We have not yet investigated any of these other algorithms. Inclusion of approximate importance sampling in the Hubbard-Stratonovich variables is straightforward, but we have not included importance sampling in the Hubbard-Stratonovich variables here.

To apply the Monte Carlo method, we use walkers that are given by the $3N$ spatial coordinates of the particles, and N 2-component complex spinors which give the spin state of each particle.

We apply the imaginary time propagator

$$\exp\left(-(H - E_{\mathrm{Trial}})\,\Delta t\right) \tag{12}$$

to our walker and sample the final configuration. This is done by dividing the propagator into a central part and a noncentral part. For small Δt, the commutator terms can be ignored, and the central propagator can be sampled to give new positions of the particles and a weight factor for the configuration. In addition, we write the noncentral part using the Hubbard-Stratonovich method. Currently, we sample the Hubbard-Stratonovich variables using the Koonin et al. approximation with probability $2/3$ a variable is zero, and with probability $1/6$ it is $\pm h$, where h is defined for each variable by Eq. (11). Importance sampling could be applied to the sampling of these variables to improve the variance.

We use the simplest possible trial function. It is a product of central two-body correlations and a Slater determinant of space and spin orbitals. We evaluate the wave function at the new space and spin positions, and apply the constrained path method by setting the weight of a walker to zero if the real part of the trial wave function is negative at the new space-spin configuration.

3. Neutron matter calculations

As a check on our method we calculated the ground state of 2 neutrons in a periodic box and in a spin singlet. Our trial function is also a spin singlet. We evaluate the potential using the nearest image convention. In this case, the tensor interaction gives no contribution and $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$ evaluates to -3. Our fixed node wave function should give the correct singlet node. A direct diagonalization or a Green's function Monte Carlo calculation with a purely central potential with the interaction given by dropping the tensor terms and setting $\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$ to -3 should therefore give the same result as our full operator result. For a box of volume 10 fm^3 using the v_6

components of the Argonne v_{18} potential, we find the correct answer to be -29.3 MeV, while or Hubbard Stratonovich method where all the operators are included gives -29.2 ± 0.2 MeV.

We have applied this method to neutron matter. As mentioned above, $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j = 1$ in this case, and we can combine these isospin terms with the corresponding term without isospin. Only the $A^{(\sigma)}$ is needed to describe the potential. We truncate the Urbana v_{14} potential by setting the terms v_7 through v_{14} to zero. We have done calculations on 38 and 54 neutrons at several densities. Our trial function contains a Slater determinant of orbitals of the form

$$\begin{Bmatrix} \sin(\boldsymbol{k}_m \cdot \boldsymbol{r}_i) \\ \cos(\boldsymbol{k}_m \cdot \boldsymbol{r}_i) \end{Bmatrix} \Xi_s(i) \tag{13}$$

where the space orbital is either a sine or cosine, the $\boldsymbol{k}_m$ are the lowest magnitude k vectors that fit in the simulation cube, and $\Xi_s(i)$ is either an up or down spinor for the particle. The determinant of orbitals is multiplied by a product of central two-body factors

$$\prod_{i<j} f(r_{ij}) . \tag{14}$$

We take $f(r)$ as the central part of the correlation operator obtained as in Ref. [12]. To evaluate Ψ_T, we overlap the orbitals spinors with the walker spinors, and evaluate the spatial orbitals and the two-body factors at the walker particle positions. The gradients of the Ψ_T and the evaluation of the full noncentral potential to calculate the energy are done similarly.

Results for some model neutron matter calculations are shown in Table 1. For comparison we show fermi hypernetted chain single operator chain (FHNC/SOC) calculations using the method of Ref. [12]. We see the agreement is fairly good showing that our method is giving reasonable physical correlations even though our trial function has no operator correlations built in. The Monte Carlo results in Table 1 have the potential set to zero at a distance of $r = L/2$ where L is the side of the box. No corrections to this number have been made. Assuming a constant density of particles for $r > L/2$, gives the central tail correction shown in the table. We have not attempted to compensate for the finite size effects from the kinetic energy terms. We have made runs at multiple time steps. The values in the table are from runs where the extrapolated time step errors are less than the statistical errors.

Table 1
The energy per particle in MeV for neutron matter using the Urbana v_6 potential, i.e. Urbana v_{14} truncated at the v_6 level, at the densities ρ shown. E_{MC} are the constrained path results described in the text using N particles. The tail correction is described in the text. $E_{\mathrm{FHNC/SOC}}$ are results using the fermi hypernetted chain single operator chain approximation of Ref. [12] for comparison

ρ (fm^{-3})	N	E_{MC}	Tail	$E_{\mathrm{FHNC/SOC}}$
0.10	38	8.8 ± 0.1	−0.15	10.92
0.10	54	8.6 ± 0.1	−0.07	10.92
0.15	38	11.8 ± 0.1	−0.52	13.46
0.15	54	12.0 ± 0.1	−0.26	13.46
0.20	38	15.5 ± 0.1	−1.17	15.94
0.20	54	15.1 ± 0.1	−0.61	15.94

4. Conclusion

In conclusion, we have given an algorithm that can allow fixed node calculations of the ground states of many nuclear systems with fairly realistic potentials. Although our trial wave functions are simple single Slater determinants with orbitals that factor into space and spin components, there is no difficulty in using good J orbitals or including more Slater determinants to improve the nodes if that proves necessary. The algorithm requires order N^3 operations at each time step, that is the same order as a straightforward implementation of the fixed node method for central potentials. The feasibility of calculating reasonable sized systems was demonstrated by our calculations for 54 neutrons.

Similar methods should allow the inclusion of some dynamical meson degrees of freedom. The Hubbard-Stratonovich method is identical to a particular formalism we would get if we included a very fast meson degree of freedom that coupled to the nucleons. This meson could be integrated out to give a potential by using the Born-Oppenheimer approximation and solving for its ground-state energy with the nucleon coordinates fixed. The meson ''coordinate'' then corresponds to the Hubbard-Stratanovich

variables. More realistic mesons could also be included.

The solution of such a coupled nucleon-meson system can be handled similarly to our calculations. For example we could include pions in our neutron matter calculations. In outline, each of the pion modes that fit in the periodic simulation cell would be given a dynamical variable that gives the magnitude of the mode. These variables satisfy a harmonic oscillator Schroedinger equation with frequency corresponding to the mode energy. These variables would correspond to the Hubbard-Stratonovich variables in our formalism above. The nucleons would couple to the pion modes proportional to

$$\boldsymbol{\sigma}_i \boldsymbol{\nabla}_i \sin(\boldsymbol{k}_m \cdot \boldsymbol{r}_i)\boldsymbol{\tau}_i \cdot \boldsymbol{T}_m \tag{15}$$

where the sine could also be cosine and gives the spatial mode of the pion. A form factor would be also need to be included. The $\boldsymbol{T}_m$ is the isospin of the mode. Notice that the eigenvectors of the A matrices in Eq. (3) are analogous to the gradient of the meson modes. Initial calculations on 1 and 2 nucleons would be required to extract the corresponding self-energy, mass correction, and static nucleon-nucleon interaction. The bulk of the interaction could be retained in the Hubbard-Stratonovich form. The propagation of this field theory is no harder in principle than our Hubbard-Stratonovich method. Semi-realistic two-pion exchange three-body interactions would be automatically included, as would retardation effects. The fixed node approximation could be used exactly as we do now. By using the first quantized harmonic oscillator Hamiltonian for the pion mode amplitudes, the bose character of the mesons is automatically included. We are currently pursuing these ideas.

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