Progress Report

Computational Methods for the Nuclear and
Neutron Matter Problems

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I. Introduction

We give a brief report of progress on the development of Monte Carlo methods for the treatment of extensive nuclear and neutron matter and of finite nuclei. A proposal is outlined for work to be carried out in a continuation of the current research.

The technical implementation of the methods proposed last year for the Monte Carlo evaluation of many-body integrals arising in the variational treatment of nuclear and neutron matter proved more difficult than anticipated. As will be described below, appropriate modifications in the Monte Carlo formalism were made and carried through for the V_4 potential. The previous method was satisfactory for V_3 and the latter calculations have been completed.

Significant progress was made in the development of the Green's function Monte Carlo method for fermion systems. For several technical reasons it proved useful to study a model nuclear few-body problem - in particular a kind of three neutron problem. This work proved successful in that a stable Monte Carlo algorithm was developed. It gave correct results for energy and wave function for a soluble (separable) test problem and reasonable results (confirmed by variational computations) for a system interacting by pairwise phenomenological potentials.

A stable GFMC algorithm for many-fermion systems has not been implemented, but ancillary studies on ^3He have advanced considerably as will be described below. In particular new methods for finding upper bounds have been devised in which Green's function methods are used. These have particular application to nuclear problems since

they are technically easier to carry out than the methods we have been investigating and may produce lower values of the upper bounds. The latter has been the outcome of the work on ^3He .

2. Progress in Variational Monte Carlo Methods

2.1 The V_3 Potential with Central Correlations

The method proposed previously for treating the V_3 potential was carried out. The trial function is a product of a determinant of plane waves with spinors by a Jastrow product containing central, possibly state dependent, correlation factors:

$$\begin{aligned} f(r_{ij}) &= \exp \left[-Ae^{-Br} (1-e^{-r/D})/r \right], \text{ for parallel spins} \\ &= \exp \left[-sAe^{-Br} (1-e^{-r/D})/r \right] \text{ for opposite spins} \end{aligned} \quad (1)$$

Results are shown in Table 1 along with integral equation results obtained by Owen⁽¹⁾ and by Pandharipande and Wiringa⁽²⁾.

2.2 The V_4 Potential with Non-central Correlations

To study the problem of noncentral correlations, we have chosen the V_4 -model of nuclear matter as a starting point. The model Hamiltonian is given by:

$$\begin{aligned} H = \frac{-\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i < j} (V_{ij}^c + V_{ij}^\sigma \vec{\sigma}_i \cdot \vec{\sigma}_j + V_{ij}^\tau \vec{\tau}_i \cdot \vec{\tau}_j \\ + V_{ij}^{\sigma\tau} \vec{\sigma}_i \cdot \vec{\sigma}_j \vec{\tau}_i \cdot \vec{\tau}_j) . \end{aligned} \quad (2)$$

where $\vec{\sigma}$ and $\vec{\tau}$ are Pauli spin and isospin matrices respectively and the V_{ij} 's are functions of $|r_{ij}|$ only. The nuclear force depends on the relative spin and isospin of the interacting particles. The replacement

$$\vec{\sigma}_i \cdot \vec{\sigma}_j = 2\pi_{ij}^{\sigma} - 1$$

$$\vec{\tau}_i \cdot \vec{\tau}_j = 2\pi_{ij}^{\tau} - 1$$
(3)

allows us to write the Hamiltonian in terms of the spin and isospin exchange operators Π^{σ} and Π^{τ} .

The V_4 model is a good starting point for two reasons.

First, the force cannot be written as a simple spatial exchange. Therefore, the eigenstates will not be well represented by the pure Jastrow wavefunction in which spatial exchange correlations are contained in the Slater determinant. An example of a term in the Hamiltonian which does not contribute in the Jastrow approximation is

$$\Pi_{12}^{\sigma} |p\uparrow\rangle |n\uparrow\rangle = |p\uparrow\rangle |n\downarrow\rangle$$

This term has changed the number of particles in each of the four spin-isospin states and is orthogonal to the Jastrow wavefunction. It is clear that the energy can be lowered by adding to the Jastrow wavefunction terms with different numbers of particles in the spin-isospin states. The lowering will be proportional to the strength of the spin + isospin potentials in the Hamiltonian.

The second reason to choose a V_4 -potential is that since it is made up of only spin and isospin potentials, the total spin and total isospin are conserved. Therefore, unlike tensor and spin-orbit forces the V_4 -model contains those features that need to be examined to develop a Monte Carlo method for nuclear matter without containing unnecessary complications. A useful trial wavefunction must contain the correlations that the potential is expected to generate. Two choices, both given by generalizing the Jastrow approximation are given by:

$$\Psi_{IP} = \{ (IP) \prod_{i < j} (f_{ij}^C + f_{ij}^\sigma \Pi_{ij}^\sigma + f_{ij}^\tau \Pi_{ij}^\tau + f_{ij}^{\sigma\tau} \Pi_{ij}^\sigma \Pi_{ij}^\tau) \} \Phi_0 \quad (4)$$

$$\Psi_{SP} = \{ S \prod_{i < j} (f_{ij}^C + f_{ij}^\sigma \Pi_{ij}^\sigma + f_{ij}^\tau \Pi_{ij}^\tau + f_{ij}^{\sigma\tau} \Pi_{ij}^\sigma \Pi_{ij}^\tau) \} \Phi_0 \quad (5)$$

here the f_{ij} 's are functions only of the distances r_{ij} and Φ_0 is a Slater determinant of plane waves and spin-isospin wavefunctions.

IP means that only independent pair terms in the operators are allowed. For example terms which include the operators $\Pi_{34}^\sigma \Pi_{37}^\sigma$ would be discarded since the operators have a common particle index. This simplifies the calculation since $[\Pi_{34}^\sigma, \Pi_{37}^\sigma] \neq 0$. The resulting correlations are fully symmetric under interchange of particle labels as required to make the full wavefunction antisymmetric. Another method to gain this symmetry is to symmetrize each operator term. This is indicated by the symmetrizing operator S in Eq. 4. We have chosen to implement the independent pair form for technical reasons. A low variance algorithm for the independent pair form can be converted to the symmetrized product form by using Monte Carlo techniques to sample among the operator permutations.

The expectation value integral can be written as

$$E_V = \frac{\int \psi_V^* H \psi_V dR}{\int \psi_V^* \psi_V dR} \quad (6)$$

where ψ_V is either ψ_{SP} or ψ_{IP} . Either one can be expressed in the form

$$\psi_V = \left(\sum_{\ell} F_{\ell} O_{\ell} \right) \Phi_0 \quad (7)$$

by expanding the product of sums of correlation functions and operators into a sum of products. The O_{ℓ} are formed by taking a product of the operators $(1, \Pi^\sigma, \Pi^\tau, \Pi^\sigma \Pi^\tau)$ - one for each pair of particles. The corresponding F_{ℓ} is then constructed by taking the product of the respective correlations $(f^C, f^\sigma, f^\tau, f^{\sigma\tau})$ for each pair.

It is necessary to antisymmetrize only the left hand ψ_v^* in the expectation value; since both H and 1 are fully symmetric the antisymmetric component of ψ_v will be projected out. It is convenient to define ϕ 's for the right and left hand ψ 's:

$$\phi_R = \text{Det} \{ \phi_i(r_j) \} \chi_i(s_i) \eta_i(I_i) \quad (8)$$

$$\text{and } \phi_L = \text{Det} \{ \phi_i(r_j) \} \chi_i(s_j) \eta_i(I_j) \quad (9)$$

where ϕ , χ , η and r, s, I are space, spin, and isospin wavefunctions and coordinates respectively. Thus in ϕ_R the spin and isospin of the particles are fixed; particles with the same spin and isospin are spatially antisymmetric.

The expectation value of the energy then becomes

$$E_v = \frac{\sum_{l,m} \int dR (\phi_L^* F_m^* O_m) H (F_l O_l \phi_R)}{\sum_{l,m} \int dR (\phi_L^* F_m^* O_m) (F_l O_l \phi_R)}$$

We define a probability distribution function

$$P(l,m,R) = \frac{|\text{Det} \{ \phi_i(r_j) \} F_l F_m|}{\int dR |\text{Det} \{ \phi_i(r_j) F_l F_m|} \quad (10)$$

and write E_v as

$$E_v = \frac{\sum_{\ell, m} \int dR P(\ell, m, R) \left\{ \frac{(\phi_L^* F_m^* O_m) H(F_\ell O_\ell \phi_R)}{P(\ell, m, R)} \right\}}{\sum_{\ell, m} \int dR P(\ell, m, R) \left\{ \frac{\phi_L^* F_m^* O_m^* (F_\ell O_\ell \phi_R)}{P(\ell, m, R)} \right\}} \quad (11)$$

This then gives a well defined problem to which the Metropolis Monte Carlo may be applied:

Spatial coordinates and operator products are drawn from

$P(\ell, \ell', R)$ by straight forward generalization of the standard Metropolis method.⁽³⁾ The most difficult problem is how to sample ℓ and ℓ' efficiently. Schemes in which ℓ and ℓ' were chosen uniformly or near each other were tried but proved to give very small acceptance ratios. A workable algorithm was developed which uses the "directed sampling method". This method picks particles at random and tries to pair or unpair them most often with those neighboring particles which tend to make $P(\ell, \ell', R)$ large. These moves are then accepted or rejected in a compensating manner. The development of a workable method of adequately sampling through the spin-isospin operators is one of the major accomplishments of our work. The calculation of the matrix elements $\langle \phi_0^* | O_\ell' H O_\ell | SI \rangle$ is also a time consuming process. In order to make the calculation of the energy practical, we must avoid recalculating this matrix element for every term in the Hamiltonian, since it would amount to doing $2N^2$ determinants, a prohibitive number.

However since each of the individual terms in the Hamiltonian contains only a two-body spin and/or isospin exchange these matrix elements can be related in terms of simple inner products. Even

so, the updating and monitoring of various pointers and matrices to facilitate the computation is rather complicated.

We have applied this method to the Reid V_4 -potential.⁽⁴⁾ This potential is constructed from the original Reid potential by turning off the tensor and spin-orbit terms.⁽⁵⁾ Preliminary results at a fermi momentum of $k_f = 1.4 \text{ f}_m^{-1}$ indicate that with pure Jastrow our energy is about 30 MeV. Our preliminary result is that the energy is not lowered by the addition of spin and isospin correlations.

3. Green's Function Monte Carlo for the Few Body Problem

To solve the Schrodinger equation⁽⁶⁾

$$H\psi(R) = E\psi(R) \quad (12)$$

we first make a shift in energy scale

$$(H + V_0)\psi(R) = (E+V_0)\psi(R) \quad (13)$$

and define Green's function for the operator on the left

$$(H + V_0)G(R, R') = \delta(R-R') \quad (14)$$

It can be proved that if E_0 is the lowest eigenvalue and if $V_0 + E_0 > 0$ then

$$G(R, R') \geq 0. \quad (15)$$

Using the Green's function the differential equation can be written as

$$\psi(R) = (E + V_0) \int G(R, R') \psi(R') dR' \quad (16)$$

This leads to an iteration

$$\psi^{(n+1)}(R) = (E+V_0) \int G(R, R') \psi^{(n)}(R') dR' \quad (17)$$

which is carried out by a Monte Carlo (random walk) algorithm. If one expands an initial function in eigenfunctions

$$\psi^{(0)}(R) = \sum_{\ell} \alpha_{\ell} \psi_{\ell}(R) \quad (18)$$

and uses the eigenfunction expansion of $G(R, R')$ one finds

$$\psi^{(n)}(R) = \sum_{\ell} \left(\frac{E + V_0}{E_{\ell} + V_0} \right)^n \alpha_{\ell} \psi_{\ell}(R) \quad (19)$$

which demonstrates convergence to the ground state, independent of the numerical value of E and the form of $\psi^{(0)}$ if the latter is not orthogonal to ψ_0 . In particular, if $\psi^{(0)}$ is an antisymmetric function then, as given by the last equation, each $\psi^{(n)}$ is also antisymmetric.

Unfortunately when the iterations are carried out by Monte Carlo the representation of $\psi^{(n)}(R)$ as a population of points contains noise, including some symmetric noise as a rule. Any symmetric component having a lower eigenvalue than the lowest fermion state will dominate asymptotically. In that case the iterations cannot be carried out unambiguously to convergence.

3.1 Alpha Particle with Malfliet-Tjon Potential

Working in collaboration with John Zabolitzky⁽⁷⁾ (of the Ruhr-Universität Bochum) we have solved numerically the Schrödinger equation for four nucleons interacting by the Malfliet-Tjon⁽⁸⁾ potential. Because this is a central force, explicit antisymmetrization of the wave function is not required and the existing Greens function Monte Carlo can be applied. First it was studied by a variational method to obtain an "importance function". GFMC was found accurate and reliable. The ground state eigenvalue is -31.3 ± 0.2 MeV and the rms point mass radius 1.36 ± 0.01 fm. These results have already been used as a benchmark for variational work by Pandharipande⁽⁹⁾ and for the coupled-cluster method by Zabolitzky.⁽¹⁰⁾

We plan to extend this work to realistic potentials using the stabilization methods described in the next section.

3.2 Model Three-fermion Problems

A method was proposed⁽¹¹⁾ to overcome the instability of GFMC integration of the fermion problem. Suppose that the wavefunction is written as a difference of two functions,

$$\psi(R) = \psi^+(R) - \psi^-(R) . \quad (20)$$

Points drawn from ψ^+ represent ψ where it is positive and ψ^- gives where negative. In general, however there may be + and - points in the same regions of configuration space. Let a pair of $\pm$ points R_+ , R_- be selected. Construct the pair of functions G^+ , G^- according to

$$G^{\pm}(R, R_+, R_-) = \begin{matrix} +\max \\ -\min \end{matrix} \left[G(R, R_+) - G(R, R_-), 0 \right] \quad (21)$$

and iterate

$$\psi^{\pm}(R) = (E + V_0) \int G^{\pm}(R, R_+, R_-) \psi^+(R_+) \psi^-(R_-) dR_+ dR_- \quad (22)$$

With the condition

$$\int \psi^+(R) dR = \int \psi^-(R) dR, \quad (23)$$

satisfied exactly by the antisymmetric state, then the new integral equation is equivalent to the Schrödinger equation.

We have carried out this procedure for some simple model three-body problems in which one pair is antisymmetrized (as if they were a pair of neutrons in the same spin state). Potentials with square attractions and repulsions were used. In one class of problems the third particle was assumed to interact with a potential depending on its distance from the center of gravity of the antisymmetrized pair. In other words,

$$V(R) = v_{12}(r_{12}) + v_{123} \left(\left| \frac{1}{2} (\vec{r}_1 + \vec{r}_2) - \vec{r}_3 \right| \right). \quad (24)$$

All potentials had the form

$$V(r) = \left\{ \begin{array}{lll} V_1 > 0 & \text{for} & r < r_1 \\ V_2 < 0 & \text{for} & r_1 \leq r < r_2 \\ 0 & \text{for} & r > r_2 \end{array} \right\} \quad (25)$$

With this potential the solution is a product of a function of r_{12} by a function of $\left| \frac{1}{2} (\vec{r}_1 + \vec{r}_2) - \vec{r}_3 \right|$. By varying the

parameters (V_1, V_2, r_1, r_2) of the potential it was possible to study the sensitivity of the method to the spectrum. In fact convergence was most rapid when the antisymmetric ground state was the first excited state of the full spectrum, as one would expect, but the method yielded stable populations and eigenfunctions and correct eigenvalues in all cases tried.

A summary of the kind of results is given in the following table:

<u>Potential</u>	<u>E_{GPMC} (MeV)</u>	<u>E_{Exact} (MeV)</u>
I	-67.5±1	-66.9
II	-73.6±1	-72.5

where the potential I(II) was chosen so that the lowest antisymmetric state was the first (second) excited state. As can be seen the energy given by the GPMC method (E_{GPMC}) is in good agreement with the known exact answer (E_{Exact}) in both cases.

Calculations were also done with a more realistic potential of the form:

$$V(R) = v(r_{12}) + v(r_{13}) + v(r_{23})$$

where $v(r)$ is given by Eqn. (25). Since no exact analytic solution to the Schrödinger equation exists, a series of variational calculations was done to determine a good trial wave function ψ_v and an upper bound to the energy E_v . An additional estimate of the fermion energy is given by

$$E_{\text{mixed}} = \frac{\int \psi_v H \psi_{\text{MC}} dR}{\int \psi_v \psi_{\text{MC}} dR} \quad (26)$$

The results of this calculation are summarized below:

<u>E_{GFMC} (MeV)</u>	<u>E_{mixed} (MeV)</u>	<u>E_v (MeV)</u>
-138.7±1.	-138.9	-133.7

The GFMC method gives a lower energy than the variational upper bound as expected. The agreement between the mixed and GFMC estimates indicates that the fermion energy is accurately calculated.

4. Green's Function Variational Methods

4.1 Transient Estimates

In spite of the asymptotic breakdown of the ordinary GFMC iteration applied to fermions, it is nonetheless possible to produce useful numerical results before the iterations reduce completely to symmetric noise. Let $\psi_T(R)$ be some antisymmetric trial function and define

$$E_n = \frac{\int \psi^{(n)}(R) H \psi_T(R) dR}{\int \psi^{(n)} \psi_T(R) dR}$$

Ceperley and Alder⁽¹²⁾ have carried out calculations of this kind for the electron gas.

If one sets

$$\psi_T(R) = \psi^{(0)}(R) \quad (27)$$

Then it is easy to prove that E_n is an upper bound to the fermion ground state

$$E_n \geq E_F \quad (28)$$

and that if the limit as $n \rightarrow \infty$ could be obtained

$$E_n \rightarrow E_F$$

A consequence of the asymptotic dominance of symmetric noise is that, for fixed computer time for each n , both numerator and denominator of the quotient that defines E_n tend toward zero. Before this happens one can obtain numerical upper bounds to E_F .

In ancillary work on ^3He we used

$$\psi_T(R) = \psi^{(0)}(R) = \exp - \sum_{i < j} u(r_{ij}) - \frac{1}{2} \lambda \sum_l \vec{G}(l) \cdot \vec{G}(l) \quad (29)$$

$$\times \det \{ \exp [i k_i \cdot (\vec{r}_j + \lambda_B \vec{G}_B(j))] \} \quad (30)$$

Both G_B and G have the general form

$$\vec{G}(l) = \sum_{i \neq l} \xi(r_{li}) \vec{r}_{li} \quad (31)$$

and ξ is a phenomenological function (with adjustable parameters) having a peak where correlations change rapidly. G introduces triplet correlations explicitly⁽¹³⁾ while G_B introduces backflow.

This function was used in variational studies of ^3He yielding an upper bound of about $-1.75 \pm .05$ K per atom. Transient estimates were carried out as well. It is not clear whether convergence has been attained but the results at $n = 30, 35, 40$ taken together yield an upper bound of

$$E_F = -2.16 \pm .05 \text{ K/atom}$$

4.2 A New Variational Method

It should be possible to carry out calculations of this kind for nuclear matter. A related method for estimating bounds which is likely to be technically easier to carry out for non-central forces is the following. Let

$$H = T + V^C + V^O \quad (32)$$

V^O being the non-central forces. Then

$$H\psi = E\psi = -B\psi \quad (33)$$

can be written

$$(T + V^C + B)\psi(R) = -V^O(R)\psi(R) \quad (34)$$

or

$$\psi(R) = - \int G^C(R, R') V^O(R') \psi(R') dR' \quad (35)$$

where G^C is Green's function for $(T + V^C + B)$ and can be obtained by existing methods. A new variational wave function $\psi_V(R)$ may be obtained starting with any antisymmetric $\psi_T(R)$:

$$\psi_V(R) = - \int G^C(R, R') V^O(R') \psi_T(R') dR' \quad (36)$$

$$E_V = \frac{\int \psi_V^*(R) H \psi_V(R) dR}{\int |\psi_V|^2 dR} \quad (37)$$

$$H\psi_V = (T + V^C + B)\psi_V + (V^O - B)\psi_F \quad (38)$$

$$\begin{aligned}
& \int \int \int \left\{ \frac{1}{2} \left[V^{O*}(R') \psi_T^*(R') + V^{O*}(R'') \psi_T^*(R'') \right] \right. \\
& \quad \left. + \left[(V^O(R) - B) V^O(R') \psi_T(R') V^O(R'') \psi_T(R'') \right] \right\} / p(R) \\
& \quad \times G(R, R'') G(R, R') p(R) dR dR' dR'' \\
E_V = & \frac{\int \int \int \left\{ V^O(R') \psi_T(R') V^{O*}(R'') \psi_T^*(R'') / p(R) \right\}}{\int \int \int \left\{ p(R) G(R, R'') G(R, R') dR dR' dR'' \right\}} \quad (39)
\end{aligned}$$

Each integral can be carried out by Monte Carlo: first sample a point R from a suitable $p(R)$. Then carry out two steps from R to R' and R to R'' respectively. Since $G(R, R')$ is symmetric, one can as easily sample R' conditional on R as R conditional on R' in the usual GFMC. Finally, averaging the braces in numerator and denominator separately and taking the quotient yields a Monte Carlo estimate of the variational energy. Certain spin-isospin sums must be done in evaluating V^O ; alternatively the sums may also be done by Monte Carlo.

5. Proposed Future Work.

- 5.1 We plan to extend our Monte Carlo variational methods to remove the restriction to the independent pair product of operators in the trial function.
- 5.2 The variational studies will be carried out for tensor forces as well.
- 5.3 We will examine new classes of trial functions that are particularly well suited for use in Monte Carlo variational calculations.
- 5.4 The treatment of few-nucleon problems by GFMC methods will be extended to non-central forces.
- 5.5 We will continue to follow the development of GFMC for the many-fermion problem and if appropriate study model systems of interest to nuclear or neutron matter.

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Table 1

Equation of State of V_3 Neutron Matter

Density n/fm^3	Variational Parameters N					$E, M_e V$				
	A	B	D	S		Monte Carlo	IP, JF ^a	IP, PB ^a	V, PB ^b	J, PB ^b
0.17	2.0	2.8	0.3	1	38	16.63±0.20	17.2	17.0	17.4	17.8
					54	16.86±0.16				
0.30	2.0	2.4	0.3	1	38	28.81±0.13	29.1	28.2	28.8	29.2
					54	28.98±0.26				
0.40	2.0	2.4	0.3	1	38	41.20±0.18	41.1	38.8	39.9	40.3
					54	41.20±0.28				
1.00	2.1	2.4	0.25	1	38	169.4 ± 1.4	---	---	---	---
					54	168.6 ± 0.7				

a. J.C. Owen, ref 1

b. Pandharipande and Wiringa, ref 2