PHYSICAL REVIEW C VOLUME 32, NUMBER 5 NOVEMBER 1985

Mirror potentials and the fermion problem

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(Received 30 May 1985)

The exact treatment of fermion systems by Monte Carlo methods has proved to be difficult. We present a new method based on the concept of a "mirror potential," which is a many-body potential that forces the Monte Carlo iteration to have a stable antisymmetric component. The potential may be determined from the wave function and, within the framework of Green's function Monte Carlo, from the random walk whose density converges to the wave function. In certain limits, the method reduces to the fixed node approximation and to transient estimation, so that it subsumes both of them. As a further consequence it offers an approximation analogous to fixed node for treating systems with noncentral forces. The method may prove to be a general one for treating random walkers with nonpositive or complex weights. In support of that we exhibit a successful calculation of a one-dimensional excited state. In this paper we explore the alternative in which the mirror potential is obtained from trial wave functions. This yields an approximation scheme that proves to be accurate in the experiments described here. We present results for a model problem in which four neutrons interact by a spin-independent potential, and compare the results with those of the fixed node method, and the method of transient estimation.

I. MANY-FERMION SYSTEMS

Green's function Monte Carlo (GFMC) has been successfully applied to solve the Schrödinger equation for a wide variety of boson systems. Successful application to fermion problems has proven to be elusive, however. In this paper we describe a new method for GFMC calculations of fermion systems. We will first review the principal methods used, the "fixed node approximation," and the method of transient estimation. The former is applicable only to systems that interact by central potentials and is, in general, of unknown *a priori* accuracy. The method of transient estimation, while essentially exact, requires exponentially increasing computing time to decrease the confidence limits as the Monte Carlo iteration is continued. The difficulty is that the iteration in question converges to the symmetric—rather than antisymmetric—ground state and in so doing suffers from an exponentially decreasing signal-to-noise ratio for fixed computing time.

It is natural to ask whether the convergence to the symmetric ground state can be inhibited. One simple possibility that is the basis of our proposed new method is to add to the Hamiltonian of the system an external many-body potential that forces the ground state to be a linear combination of symmetric and antisymmetric components, of which the latter is the correct many-fermion ground state. We term this additional potential a "mirror potential" because it acts differently on the positive and negative random walkers, constraining them to stay predominantly in separate parts of coordinate space, namely those where the fermion ground state is respectively positive and negative.

The required potential is obtained from the ground state wave function; we show below how it may be obtained in principal from the random walk that solves the Schrödinger equation.

We show also that in suitable limits, the method reduces to the fixed node approximation and to transient estimation. Thus it provides a coherent theoretical framework for discussing and understanding both. Furthermore, and we believe that this will prove to be important, it offers a method for treating quantum systems with noncentral forces by an approximation analogous to the fixed node. It may prove still more generally to be a method for treating walkers with complex weights.

This paper is devoted to the general introduction to the ideas of the mirror potential and to the exploration in model problems. We stress the use of approximate mirror potentials. That is, instead of computing the mirror potential from the exact and unknown ground state, we use trial functions of the kind used in both the fixed-node approximation and in transient estimation. We find that its accuracy is comparable to the fixed node and that it may yield lower energy.

Green's function Monte Carlo produces the solution of the Schrödinger equation as a set of points in configuration space distributed with a probability density ϕ_n which converges toward ϕ_0, the ground state wave function of the system. The GFMC method,[1] in essence, consists of choosing a set of points and iterating the equation

$$\Psi_{n+1}(R)=(E+V_0)\int G(R,R')\Psi_n(R')dR' . \quad (1.1)$$

$G(R,R')$ is not known analytically, but may be sampled, for example, from the equation

$$G(R,R')=G_u(R,R')+\int_D G(R,R'')[U(R'')-V(R'')] \times G_u(R'',R')dR'' + \int_D G(R,R'')[-\nabla G_u(R'',R')\cdot\hat{\mathbf{n}}]dS , \quad (1.2)$$

where G_u is the solution for the Green's function within a

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domain D for a constant potential U, and is known analytically.[2] This requires an ancillary walk whose expected density develops the Green's function.

This method is difficult to apply to fermion systems, because the wave function must be antisymmetric with respect to the interchange of the coordinates of any two identical particles. Superficially, the convergence of Eq. (1.1) to the lowest state not orthogonal to Ψ_0 guarantees that an antisymmetric Ψ_0 will generate a sequence converging to the lowest antisymmetric state, the fermion ground state. This is entirely true, but beside the point, since a Ψ_0 that can be sampled as a density function is necessarily positive and has nonzero overlap with the Bose ground state.

The difficulty discussed in the last paragraph is, again superficially, easily remedied. We must use positive densities and therefore write the wave function $\Psi(R)$ as the difference of two densities $\phi(R)$:

$$\Psi_n^A(R)=\phi_n^+(R)-\phi_n^-(R)\ , \tag{1.3}$$

where each $\phi_n^{\pm}$ is itself positive and can be thought of as derived from a density of random walkers. Then Eq. (1.1) becomes

$$\Psi_{n+1}^A(R)=(E_0+V_0)\int G(R,R')[\phi_n^+(R')-\phi_n^-(R')]dR'\ , \tag{1.4}$$

which may correctly be derived from the pair of recurrences

$$\phi_{n+1}^{\pm}(R)=(E_0+V_0)\int G(R,R')\phi_n^{\pm}(R')dR' \tag{1.5}$$

for the densities alone. Equation (1.5) describes independent random walks that separately give densities for the positive or negative parts of the fermion ground state.

There is, of course, no unique way of decomposing an antisymmetric function into a difference of two positive functions. An acceptable choice is

$$\begin{aligned}\phi_0^{A\pm}(R)&=\max[\pm\phi_0^A(R),0]\\&=\tfrac{1}{2}\phi_0^A(R)\pm\tfrac{1}{2}\,|\,\phi_0^A(R)\,|\ .\end{aligned} \tag{1.6}$$

In the second form, it is manifestly a sum of an antisymmetric and a symmetric function. When we consider the nature of the convergence as in Eq. (1.1), we keep the leading symmetric and antisymmetric terms:

$$\phi_n^{\pm}(R)\rightarrow c_{S0}\Psi_{S0}(R)\pm\left[\frac{E_{S0}+V_0}{E_0^A+V_0}\right]^n\Psi_0^A(R)\ , \tag{1.7}$$

where for clarity we denote the (boson) ground state as Ψ_{S0}. The ratio that appears in the second term is less than one, so the contribution of the fermion state decreases geometrically.

A. The method of transient estimates

Although the coefficient of the interesting (i.e., antisymmetric) part of Eq. (1.7) decays, it is possible to project it out. By multiplying by any antisymmetric function, $\Psi_T^A(R)$, and integrating, we annul the leading term:

$$\int\Psi_T^A(R)\phi_n^+(R)dR\rightarrow\left[\frac{E_{S0}+V_0}{E_0^A+V_0}\right]^n c_0^A\langle\Psi_T^A\,|\,\Psi_0^A\rangle\ . \tag{1.8}$$

If Ψ_T^A is a suitable fermion trial function, then $H\phi_T^A$ is antisymmetric and well behaved, so that

$$\int[H\Psi_T^A(R)]\phi_n^+(R)dR\rightarrow\left[\frac{E_{S0}+V_0}{E_0^A+V_0}\right]^n c_0^A\langle H\Psi_T^A\,|\,\Psi_0^A\rangle \tag{1.9}$$

and

$$\frac{\int H\Psi_T^A\phi_n^+dR}{\int\Psi_T^A\phi_n^+dR}\rightarrow\frac{\langle\Psi_T^A\,|\,H\Psi_0^A\rangle}{\langle\Psi_T^A\,|\,\Psi_0^A\rangle}=E_0^A\ . \tag{1.10}$$

In a Monte Carlo calculation in which a population of random walkers represents the density (here ϕ_n^+), the integrals that appear in the last equations are estimated by sums of the function Ψ_T^A and $H\Psi_T^A$ evaluated at the positions of the walkers. The Monte Carlo estimator for Eq. (1.10) is thus

$$\frac{\sum_k[H\Psi_T^A(R)]_{R=R_k}}{\sum_k[\Psi_T^A(R)]_{R=R_k}}\rightarrow E_0^A\ . \tag{1.11}$$

The method seems then to be straightforward and natural for Monte Carlo treatment. Unfortunately a deeper look reveals the flaw: If we examine the variance of Monte Carlo estimates of the integrals which appear in Eqs. (1.8) and (1.9), we observe that they have the form

$$\text{variance}\int\Psi_T^A\phi_n^+dR\propto\int(\Psi_T^A)^2\phi_n^+dR-\left[\int\Psi_T^A\phi_n^+dR\right]^2\ . \tag{1.12}$$

But the square of the antisymmetric function Ψ_T^A is symmetric; therefore in the variance the symmetric leading team is not projected out. The result is that as the signal from Eq. (1.8) becomes small, the noise remains asymptotically constant. The signal to noise ratio decreases. If one attempts to overcome this by letting the population grow, the time grows geometrically in execution time. It cannot be predicted in advance whether the relaxation to the ground state will be seen before the Monte Carlo error grows too large. Nevertheless, useful results have been obtained by this method. Ceperley and Alder[3] presented data for the electron gas in which their energies appear to have stabilized. These results have proved consistent with subsequent approximate many-body calculations.

Schmidt[4] pointed out that if Ψ_T^A in Eqs. (1.8)—(1.11) is set equal to Ψ_0^A, then each quotient that appears in Eq. (1.10) is an upper bound to E_0^A, the fermion ground state. Using this idea, he and his collaborators obtained a series of upper bounds for a 38 particle system of unpolarized ^{3}He. It was not clear whether they had converged, but the last values were combined to yield an upper bound of $E_0^A\leq-2.20\pm0.05K$. More recently,[5] calculations of a 54 particle system converged to yield a ground state energy of $E_0^A\leq-2.25\pm0.04K$.

B. The fixed node approximation

The exact fermion wave function $\Psi_0^A(R)$ changes sign on application of an odd permutation among indistinguishable particles (here assumed to have the same spin). It is also continuous, and consequently it vanishes on some surface. That is, for an N body system $\Psi_0^A=0$ on manifolds of $3N-1$ dimensions. In general these manifolds cannot be predicted solely on the basis of symmetry principles; they are the outcome of the solution of the problem. This is unfortunate, for were they known in advance, the Schrödinger equation could be solved by the Green's function methods discussed before, using $\Psi_0^A=0$ as a boundary condition. In the absence of such an exact condition, one can use the boundary condition that the wave function vanish on the nodal surface of some approximation $\Psi_T^A(R)$ to the ground state function. This was first used by Anderson.[6] It is now known (cf. Ref. 7) that the energy obtained lies above the exact ground state, below that obtained from the variational method using Ψ_T^A as trial function, and is second order in the difference $\Psi_T^A-\Psi_0^A$. Ceperley[8] obtained an energy of $-2.06\pm0.05K$/atom for unpolarized ^{3}He in this way. The method has also been applied to few-electron[9] and many-electron[3,10] systems. Results obtained have generally been useful, especially those for the equation of state of condensed hydrogen found by Ceperley.[10]

C. Mirror potential methods

As noted previously, there is no unique way of decomposing the antisymmetric wave function into a difference of two positive functions. The methods described previously represent the two extremes for the choice of this decomposition. In the transient estimation method, the ϕ^+ and ϕ^- populations converge to identical symmetric distributions, while for the fixed node method ϕ^+ and ϕ^- have no overlap. The mirror potential method is a generalization of these techniques, encompassing them as special cases.

By writing the coupled equations for Ψ^+ and Ψ^-:

$$\{H(R)+C(R)\Psi^-(R)\}\Psi^+(R)=E\Psi^+(R)\,, \tag{1.13}$$

$$\{H(R)+C(R)\Psi^+(R)\}\Psi^-(R)=E\Psi^-(R)\,, \tag{1.14}$$

it is possible to create distinct stable populations for Ψ^+ and Ψ^- and retain the property that the difference $\Psi=\Psi^+-\Psi^-$ satisfies the original Schrödinger equation. Interpreting $C\Psi^-$ as a repulsive "mirror" potential for Ψ^+ (and $C\Psi^+$ as a repulsive potential for Ψ^-), we may solve for Ψ^+ and Ψ^- and subtract to obtain Ψ. As long as we choose $C(R)$ to be a symmetric function, $\Psi^+(PR)=\Psi^-(R)$ for any odd permutation P, and the resulting wave function will be antisymmetric.

By adjusting the strength of $C(R)$, Ψ^+ and Ψ^- may be constrained to be large in distinct and well-separated regions, namely those in which $\Psi^+-\Psi^-$ is, respectively, positive and negative. This is necessary in order to reduce the statistical error associated with the calculation. On the other hand, $C(R)$ must not be too large. Imagine a procedure in which an approximate solution is introduced for $\Psi^-(R)$ in Eq. (1.13), and the equations for Ψ^+ and Ψ^- iterated. Very large values of $C(R)$ will inhibit the motion of the nodal surface (where $\Psi^+=\Psi^-$), precisely as in the fixed node method.

We have tested the mirror potential method in two simple problems; obtaining solutions for the lowest antisymmetric states of the one-dimensional infinite square well and the three-dimensional harmonic oscillator. In these calculations our knowledge of the wave functions Ψ^+ and Ψ^-, and consequently of the mirror potential, is limited to distributions of points $\{R_k\}$. Thus, in order to evaluate the mirror potential, one may use the fact that the wave function is a solution of Eq. (1.1), and therefore

$$\Psi^-(R)=\sum_k G(R,R_k)=\sum_k\sum_l G_u(R,R_{k,l})\,, \tag{1.15}$$

where the first sum extends over all of the points in the Ψ^- distribution, and the sum over l indicates a sum over all points in the random walk which determines the full G from G_u [Eq. (1.2)]. It is not obvious that this type of walk will produce the correct solution, since the potential is determined stochastically at each point of the walk. However, by expanding Eq. (1.2) in powers of $G_u(R,R')$, it is apparent that the solution remains exact as long as succeeding evaluations of the mirror potential are independent. In general, $G(R,R')$ is relatively short ranged, and thus many configurations may be required for successful calculations in many-dimensional systems.

We have used this method of deriving a repulsive "mirror" potential for calculating states of the one-dimensional square well and the three-dimensional harmonic oscillator. The wave functions Ψ^+ and Ψ^- for the one-dimensional infinite square well are plotted in Fig. 1. The solutions for $\Psi=\Psi^+-\Psi^-$ are stable over a wide range of constant values for c, and are independent of the initial distribution of configurations.

In addition to calculating antisymmetric ground states, the mirror potential method may be used to calculate the excited states of a system. As an example, we have calculated the first symmetric excited state of the one-dimensional infinite square well. In this calculation, the initial set of ϕ^+ walkers are concentrated in the center of the well, and a set of ϕ^- walkers is concentrated near the

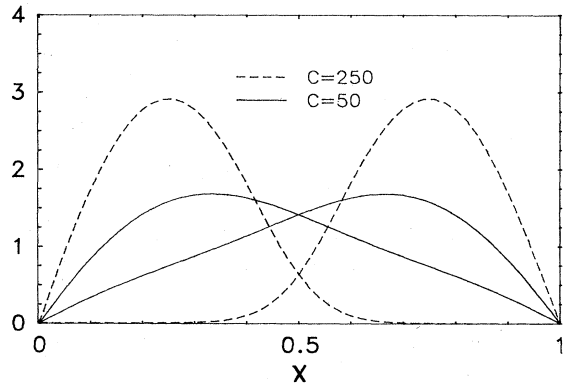

FIG. 1. The solutions of the mirror potential equation in a one-dimensional square well for two different constant values of C (arbitrary units).

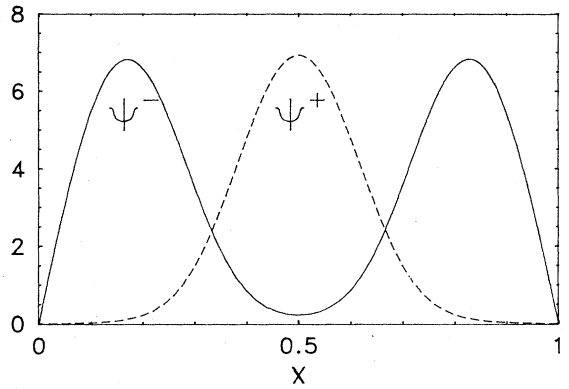

FIG. 2. The solution of the coupled mirror equations for the lowest symmetric excited state of a one-dimensional square well.

edges. The wave functions Ψ^+ and Ψ^- are indicated in Fig. 2. We wish to simply iterate Eq. (1.1) in order to obtain these solutions for the excited state. Two additional prescriptions are necessary, however, in order to obtain the exact solution for this state. First, unlike the antisymmetric ground state problem, the relative normalization of the ϕ^+ and ϕ^- populations is not known beforehand. The ratio can easily be determined, however, since for the correct value, the ratio remains constant as the Green's function equation is iterated.

Also, the solution of the equation must be symmetrized after each iteraction. This is easily accomplished, for example, by randomly choosing each configuration as either itself or its mirror image. If this is not done, fluctuations in the two populations will eventually allow them to decay into the antisymmetric ground state.

The mirror potential method, as presented, makes exact calculations of fermion systems possible for few-body systems. It may be difficult to handle many-body problems in this manner, however, since it may be difficult to obtain a density of points sufficient to determine the mirror potential. Later, in this paper, we present approximations to the mirror potential method. First, we briefly discuss the use of nonlocal mirror potentials to overcome this problem, that is, to extend the effective range of the kernel in Eq. (1.15).

D. Generalizations of mirror potentials

It is possible to generalize further the concept of mirror potentials in several ways. We describe two such generalizations here, with the expectation that more complete descriptions will follow upon further studies.

The major difficulty associated with the exact mirror potential method is the short range nature of the Green's function which is used to evaluate the mirror potential [Eq. (1.15)]. In order to overcome this difficulty, it is useful to consider the possibility of using a mirror potential which is nonlocal in nature. That is, we may replace the earlier equations [(1.13) and (1.14)] for Ψ^+ and Ψ^- by

$$H\Psi^+(R)+\int s(R,R',R'')\Psi^-(R')\Psi^+(R'')dR'dR'' = E\Psi^+(R) \quad (1.16)$$

and

$$H\Psi^-(R)+\int s(R,R',R'')\Psi^+(R')\Psi^-(R'')dR'dR'' = E\Psi^-(R) . \quad (1.17)$$

The difference $\Psi^+-\Psi^-$ again satisfies the Schrödinger equation, and by requiring $s(R,R',R'')=s(R,R'',R')$ we ensure that $\Psi^+(R)=\Psi^-(PR)$ for any odd permutation P. The motivation for introducing a nonlocal interaction is to allow for a more effective sampling of the mirror potential, since the kernel $s(R,R',R'')$ spreads the repulsive effect of the points in Ψ^- over a larger region.

A nonlocal interaction can be introduced into the GFMC method by writing an equation analogous to Eq. (1.2). With the inclusion of a nonlocal interaction, another element is introduced into the random walk. The potential is no longer simply an absorbing term in the diffusion equation, but can itself introduce steps in the walk.

An important consideration when treating nonlocal interactions is that the Green's function $G(R',R)$ may no longer be positive definite. The sign of the Green's function may change at long distance if, for example, the nonlocal interaction is repulsive and has a long range. Nevertheless, such a system may be treated successfully as long as the Green's function is predominantly positive. We have successfully treated several simple test problems with this method, but further work is required in order to test its practicality for more difficult problems.

Another important generalization of the mirror potential is useful to treat systems involving spin-dependent interactions. In such a system, the potential V may be divided into spin-independent and spin-dependent parts, V^c and V^s, respectively. The Green's function equation [Eq. (1.1)] may then be rewritten as

$$\Psi_{(n+1)}(R)=\int G(R,R')[E-V^S(R')]\Psi_{(n)}(R')dR' . \quad (1.18)$$

The spin-dependent part of the interaction will introduce transitions between different spin components of the wave function and may also introduce changes in sign. Even for systems which are predominantly symmetric in spatial coordinates, such as s-shell nuclei, this can lead to the same difficulties as in the fermion problem. That is, there will be large cancellations between walkers of opposite signs.

A mirror potential term may be introduced into the Schrödinger equation in order to overcome this difficulty. The mirror potential for Ψ^+ may take the form

$$\langle a \mid V(R) \mid b \rangle = C_a(R)\Psi_a^-(R)\delta_{a,b} , \quad (1.19)$$

where a and b label the spin states. This interaction retains the property that $\Psi^+-\Psi^-$ solves the original Schrödinger equation.

II. APPROXIMATE METHODS

By replacing the exact wave function $\Psi^\pm$ with a trial function $\Psi_T^\pm$ in the expression for the mirror potential, we can solve the equation for $\Psi^\pm$ using standard GFMC techniques. The wave function obtained in this manner is an accurate approximation to the exact wave function.

The exact solution for $\Psi^\pm$ can be chosen to be of the

form $\Psi^S \pm \Psi^A$, where S and A indicate symmetric and antisymmetric components, respectively. Inserting this expression into the Ψ^+ equation and solving for $C(R)$ yields the following expression for the mirror potential:

$$C(R)\Psi^-(R)=\frac{[E-H]\Psi^S(R)}{\Psi^S(R)+\Psi^A(R)}\ , \tag{2.1}$$

where we have used the fact that $[E-H]$ acting on the exact antisymmetric state yields zero. In order to approximate the mirror potential, we may replace Ψ^S and Ψ^A by trial functions Ψ_T^S and Ψ_T^A, and the unknown eigenvalue E by a constant E^*.

Once this approximation is made, the analytic forms for Ψ_T^S and Ψ_T^A yield an easily calculable mirror potential, and the resulting Schrödinger equation can be solved to obtain a wave function Ψ^+ and two estimators for the energy, the eigenvalue E_e of the equation, and the mixed estimator E_m, defined as

$$E_m=\frac{\int \Psi_T^A H\Psi^+ dR}{\int \Psi_T^A \Psi^+ dR}\ . \tag{2.2}$$

In order to obtain an accurate approximation to the exact wave function and energy, E^* should be adjusted until the eigenvalue $E_e=E^*$. When this condition is satisfied, $E_m=E^*=E_e$. Actually, E_m varies only in second order in the differences between E_e and E^*, so it is numerically most accurate.

The trial function Ψ_T^A should be taken to be an accurate variational wave function. The choice of Ψ_T^S is not tightly constrained, but it should satisfy two general conditions. First, $\Psi_T^S+\Psi_T^A$ should be positive everywhere, as this is required for a finite mirror potential. Second, $(E^*-H)\Psi_T^S$ should be predominantly positive, in order that the mirror potential be repulsive.

We have found that a satisfactory choice for Ψ_T^S is

$$\Psi_T^S=[(k^A\Psi_T^A)^2+(k^B\Psi_T^B)^2]^{1/2}\ , \tag{2.3}$$

where Ψ_T^B is a symmetric state of low energy and k^A and k^B are constants. The parameters k^A and k^B may be chosen to adjust the strength of the antisymmetric component of Ψ_T^+. With this choice Ψ_T^+ is positive definite, and the mirror potential will be predominantly repulsive.

Examining the consequences of this approximation, it is apparent that any choice of Ψ_T^+ with the correct antisymmetric component will give the exact wave function and energy. Furthermore, we will show that if E^* is adjusted so that $E^*=E_E$, the error in E_e is second order in the error in Ψ_T^A, and that E_e is less than the variational energy E_V obtained with Ψ_T^A:

$$E_V=\frac{\int \Psi_T^A H\Psi_T^A dR}{\int \Psi_T^A \Psi_T^A dR}\ . \tag{2.4}$$

To prove this, compare the two Hamiltonians:

$$H_1=H+\frac{[E^*-H](\Psi_T^S)}{\Psi_T^S+\Psi_T^A}\ , \tag{2.5}$$

$$H_2=H+\frac{[E^*-H](\Psi_T^S+\Psi_T^A)}{\Psi_T^S+\Psi_T^A}\ . \tag{2.6}$$

H_1 is the mirror potential Hamiltonian and H_2 is a Hamiltonian that has as its solution the trial wave function Ψ_T^+ and an eigenvalue E^*. Setting $E^*=E_V$ and calculating the expectation value of H_1 with the eigenfunction of H_2 yields an energy of E_V. Since the solution of H_1 must have an energy less than or equal to this expectation value, the point at which $E^*=E_e$ must lie at or below the variational energy E_V.

It is also possible to show that the energy at which $E_e=E^*$ is an upper bound to the exact energy in first order perturbation theory in the difference H_1-H_2, or equivalently, in the difference between Ψ_T^A and the exact Ψ^A. If we compare H_1 and H_2 and take E^* to be the exact fermion energy E_f, then to first order the eigenvalue of H_1 is

$$E=E_f+\frac{(E_V-E_f)(\int \Psi_T^{A^2} dR)}{\int (\Psi_T^{A^2}+\Psi_T^{S^2})dR}\ , \tag{2.7}$$

which is greater than the exact fermion energy. Therefore, the point at which $E^*=E$ lies between the exact energy E_f and the variational energy E_V.

Our numerical experiments with simple systems confirm these properties. It should be noted, though, that for very poor choices of Ψ_T^S (those that give rise to strong attractive regions for the mirror potential) it may not be possible to find a value of E^* such that $E_e=E^*$. In general, we find that the approximate mirror potential gives quite good results, even for relatively poor choices of antisymmetric trial functions.

Once again, this method can be easily extended to excited states. The trial function used to generate the mirror potential may have any type of nodal structure, and the difference of the two populations will have this same structure. As in the exact method, the mirror potential should be adjusted to ensure that the Ψ^+ and Ψ^- populations grow at the same rate.

III. FOUR-NEUTRON CALCULATIONS

In order to test the approximate mirror potential method, we have studied a system of four neutrons interacting through a central potential. The potential is the Mafliet-Tjon[11] MTV central potential, multiplied by a constant strength factor of 1.3 that ensures that the system is bound.

Fixed node and transient estimation calculations have been performed as well, in order to provide a basis of comparison. In each of these calculations, a trial wave function is a necessary starting point.

We used a trial function of the form

$$\Psi=\left[\prod_{i<j} f_k(r_{ij})\right]\Phi\ , \tag{3.1}$$

where f_k is a pair correlation function having one of two forms depending upon whether the two neutron spins are parallel or antiparallel. The function Φ gives the correct angular momentum for the state of interest; for the $L=0$ state it is simply $\mathbf{r}_{12}\cdot\mathbf{r}_{34}$ (where the pairs 1,2 and 3,4 have parallel spins).

The correlation functions are made to satisfy two-body

Schrödinger equations with parametrized potential terms $\lambda(r)$:

$$\left[\frac{-\hbar^2\nabla^2}{m}+v(r)+\lambda(r)\right]f(r)\Phi_{ij}=0\ , \tag{3.2}$$

with $\Phi_{ij}=1$ for opposite spins (s wave) and $r_{ij}Y_1^m(r_{ij})$ for parallel spins. The long-range parts of the correlations were chosen to have the correct properties as the system separates into two "deuterons." Thus, $\lambda(r)$ for the s-wave correlations is taken to be

$$\lambda(r)=\alpha/[1+\exp((r-r_t)/\mu)]+E_a\ . \tag{3.3}$$

The parametrization of $\lambda(r)$ for parallel spins is

$$\lambda(r)=\alpha'/[1+\exp((r-r_t)/\mu)] + \frac{\hbar^2}{m}\left[\frac{3}{4r^2}-3\frac{\gamma}{r}+\gamma^2\right](1+e^{-(r/c)^2})\ . \tag{3.4}$$

The variational parameters are E_a, γ, r_t, μ, and c; α and α' are adjusted so that $rf(r)\Phi_{ij}=0$ at $r=0$.

This form of trial function proved superior to several others that were investigated. Even so, better functions could undoubtedly be obtained. This is not necessarily an advantage when attempting to compare various GFMC methods, however, since all methods are exact given an exact trial function.

For the $L=0$ state of the four-neutron system, we obtain a variational energy of -8.75 ± 0.1 MeV. Thus, the system is very loosely bound, since with this same interaction, the ground state of two neutrons has an energy of -3.0 MeV. We have also calculated the $L=1$ and 2 states variationally. The $L=2$ state energy is -6.54 ± 0.1 MeV, while the $L=1$ state was not bound with this variational wave function.

The GFMC studies of this system were performed for the $L=0$ ground state only. This four-neutron system is very loosely bound and has a relatively simple nodal structure, so it is plausible that a fixed node calculation should give an accurate answer. That is, the exact position of the nodes should have relatively little effect upon the energy. Our fixed node calculations yield an energy of -9.36 ± 0.02 MeV, a 0.6 MeV increase in binding over the variational result. A summary of results obtained from each of the calculations is given in Table I.

Several sets of transient estimation studies have also been performed for the four-neutron system. However, these calculations are very difficult, since the alpha particle is very strongly bound by this interaction, with a binding energy of greater than 65 MeV. Consequently, transient estimation calculations are quickly dominated by noise, because of the rapid decay into the symmetric ground state.

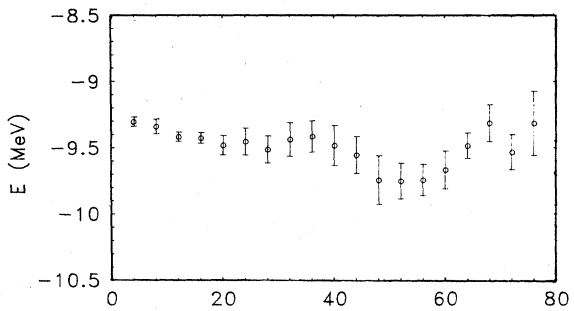

FIG. 3. The energy of transient estimation calculations versus iteration beginning with the fixed node solution. The values at each generation are not statistically independent.

In order to ensure that a true upper bound to the energy is obtained, a transient estimation iteration must begin with the same antisymmetric function used to project out the antisymmetric part of the density of walkers. However, the bound that we obtain from this calculation, -9.23 ± 0.07 MeV, is not as low as the fixed node result. This is a result of the fact that the statistical error associated with the calculation increased rapidly as the Green's function equation was iterated, and it was not feasible to iterate the solution with enough accuracy to demonstrate convergence.

We have also performed transient estimation calculations starting from the solution of the fixed node problem. The energy obtained with this method is -9.50 ± 0.07, and although it cannot be proved to be an upper bound to the energy, this result is probably the best available indication of the correct total energy. The calculated energy as a function of the number of iterations is given in Fig. 3, and the increase in noise is readily apparent. There is a definite increase in binding obtained by the transient estimation technique, but this increase is only 0.15 ± 0.07 MeV, another indication that the fixed node result is quite accurate.

Finally, the binding energy of this system has been calculated with the approximate mirror potential technique. The results are summarized in Table I, and the input mirror potential parameters for the various calculations are given in Table II. The initial calculations were performed as described above. For this calculation (listed as 4A in

TABLE I. Results.

No.	Type	$\langle H\rangle$	$\langle V\rangle$	E_e
1	variational	-8.75 ± 0.10	-83.4 ± 1.0	
2	fixed node	-9.36 ± 0.02	-81.7 ± 0.3	
3	transient estimation	-9.50 ± 0.07	-80.5 ± 0.7	
4A	mirror potential	-9.43 ± 0.05	-83.3 ± 0.8	-9.07 ± 0.01
4B	mirror potential	-9.37 ± 0.04	-81.3 ± 0.6	-9.18 ± 0.02
4C	mirror potential	-9.28 ± 0.02	-82.2 ± 0.4	-9.26 ± 0.05
4D	mirror potential	-9.31 ± 0.03	-81.4 ± 0.4	-9.06 ± 0.10

TABLE II. Mirror potential parameters.

No.	E^a	B^a	k^A	k^B
4A	−9.0		2.0	2.0
4B	−9.0	−65.0	1.0	250.0[a]
4C	−9.5	−65.0	1.0	250.0[a]
4D	−9.0	−65.0	1.5	500.0[a]

[a] Ψ_B is a product of s-wave correlations, k_B in arbitrary units.

the table), the wave function Ψ^B was taken as the simple product of pair correlations without the antisymmetrizing function Φ. This calculation yielded an estimate for the energy of -9.43 ± 0.05 MeV, an encouraging result.

We also attempted to use a wave function Ψ^B much closer to the symmetric ground state wave function of the system, in order to measure the sensitivity of the method to the choice of symmetric wave function. The product of opposite spin (s-wave) Jastrow correlations is a reasonable approximation for the alpha particle ground state, and we used it for the second set of calculations. However, this wave function has a much smaller radius than that of the antisymmetric state, and the mirror potential will become infinite for $k^A=1$ at large distances, unless the antisymmetric trial wave function is exact in that region. Therefore, the quantities $H\Psi^A/\Psi^A$ and $H\Psi^B/\Psi^B$ in the $H\Psi_S$ term of the expression for the mirror potential,

$$\frac{H[(k^A\Psi^A)^2+(k^B\Psi^B)^2]^{1/2}}{[(k^A\Psi^A)^2+(k^B\Psi^B)^2]^{1/2}} = \frac{H\Psi^A}{\Psi^A}\frac{(k^A\Psi^A)^2}{(k^A\Psi^A)^2+(k^B\Psi^B)^2} + \frac{H\Psi^B}{\Psi^B}\frac{(k^B\Psi^B)^2}{(k^A\Psi^A)^2+(k^B\Psi^B)^2}+\cdots, \tag{3.5}$$

are replaced by the constants B^* and E^*, respectively. The remaining terms, involving $\nabla\Psi^A\cdot\nabla\Psi^B$, are calculated as before. With this approximation, the mirror potential is well behaved even in regions where Ψ^B is very small.

All of these calculations gave similar, although not identical, results. The results are fairly insensitive to choices of E^* or the constants k^A and k^B.

IV. SUMMARY

The mirror potential method provides a coherent framework for studying various methods of treating fermion systems. The initial results of our calculations are encouraging, and several specific areas merit further investigation.

In particular, calculations with approximate mirror potentials appear very promising. The approximate scheme presented here provides accuracy comparable to the fixed node method in this problem. This is a favorable result, since this is a loosely bound system and the fixed node result is quite good. It would be useful to employ the various fermion GFMC schemes for several systems, in order to determine how strongly our results are dependent on the fact that this is a very loosely bound system.

Of even greater interest is the possibility of developing corrections to this approximate method. These corrections will appear as changes in the mirror potential due to the difference between the trial wave function and the solution of the approximate mirror potential equation, and would allow one to obtain much greater accuracy in the solution of the Schrödinger equation.

Finally, the possibility of applying GFMC to systems with nonlocal and spin-dependent interactions is very intriguing. Green's function Monte Carlo could be applied in many areas of physics where calculations have been impractical. Such calculations would be very valuable in areas such as nuclear systems with realistic interactions.

ACKNOWLEDGMENTS

We would like to thank M. A. Lee, R. M. Panoff, K. E. Schmidt, and Paula Whitlock for valuable suggestions and discussions during this work. This work was supported in part by the Applied Mathematical Sciences subprogram of the Office of Energy Research, U.S. Department of Energy, under contract number DE-AC02 76ER03077, and by the Division of Nuclear Physics of the Office of High Energy and Nuclear Physics, U.S. Department of Energy, under contract number DE-AC02-79ER10353.

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