Green's function Monte Carlo study of light nuclei

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The first Green's function Monte Carlo calculations of $A=3$ and 4 nuclei with spin-dependent interactions are reported. Green's function Monte Carlo methods for calculating properties of coupled channel quantum systems are described in detail, including both exact and approximate schemes. Results are presented for $A=3$ and 4 nuclei with a $V6$ interaction. For the triton, the Green's function Monte Carlo calculations are compared with Faddeev and variational methods. Green's function Monte Carlo calculations of the alpha particle provide the first test of variational methods for systems with spin-dependent interactions. For this interaction, variational methods underestimate the binding energy of the alpha particle by ≈ 2 MeV. Other ground state properties of light nuclei have also been determined. Implications of these results for more realistic interactions are discussed, along with the possibility of future extensions of Green's function Monte Carlo methods to treat momentum dependent and three nucleon interactions.

I. INTRODUCTION

The Green's function Monte Carlo[1-3] (GFMC) method has proven to be very successful in determining ground state properties of a wide variety of quantum many-body systems, including solid and liquid helium[4-7] and atomic and molecular[3,8] systems. However, it has only been used to treat systems with simple state independent interactions,[9,10] severely limiting its applicability in areas such as nuclear physics, where the spin dependence of the interactions is extremely important.

In this paper, Green's function Monte Carlo methods to treat systems with a strong spin dependence are introduced. An exact method (which may involve transient estimation[6,11]) and a "fixed phase" method (a generalization of the fixed node[8,11] method used for spin-independent interactions) are described. These techniques are outlined in the first section of the paper, and a simple coupled harmonic oscillator problem is presented to illustrate the method.

In Sec. II, the application of the GFMC method to light nuclei is discussed. Previously, $A=3$ nuclei have been calculated with variational,[12-14] Faddeev,[15,16] and coupled cluster[18] methods. For $A=3$ nuclei, it is possible to include enough channels to perform essentially exact Faddeev calculations. For $A=4$, however, both Faddeev[17] and coupled cluster[18] methods are extremely difficult. As a consequence, variational calculations are the principal method used for light nuclei with $A>3$. The error inherent in these calculations is not known, so the development of other methods is very important.

Results for the triton with the ATS-3 (Ref. 19) potential are presented in the Sec. III. This potential involves only central and spin-spin interactions, so it is conceptually simple. Both exact and the approximate fixed phase methods are employed for this problem. A comparison of the results yields information concerning the deficiencies of the variational wave function.

Results of calculations of ^{3}He and ^{4}He nuclei for a $V6$ (1, $\sigma\cdot\sigma$, $\tau\cdot\tau$, $\sigma\cdot\sigma\tau\cdot\tau$, S, and $S\tau\cdot\tau$) interaction are also presented in Sec. III. These results are compared with Faddeev calculations of the triton and variational calculations for both ^{3}He and ^{4}He nuclei. The accuracy of the variational calculations is discussed with regard to implications for more realistic two and three nucleon interaction models.

Finally, future generalizations and applications of GFMC methods are discussed in Sec. IV. Important generalizations of these methods include more realistic nuclear interactions, such as $L\cdot S$ and three body interactions. Other applications include semirelativistic and nonrelativistic constituent quark models.

II. GFMC METHODS FOR SPIN DEPENDENT INTERACTIONS

Green's function Monte Carlo methods involve a series of random walks constructed to solve the Schrödinger equation for the ground state. Two types of methods are commonly employed, the domain[3] Green's function method and the short time[20] approximation. The domain GFMC method has several advantages, the principal one being that no time step errors are introduced, and consequently no extrapolation to zero time step is necessary. On the other hand, short time methods are extremely simple, and this is a compelling virtue when studying complex spin-dependent systems. Consequently, this work will be undertaken in the framework of the short time approximation.

In this method, random walks are constructed to solve the Schrödinger equation in imaginary time

$$\Psi(\tau)=\exp(-H\tau)\Psi(0)\ , \tag{1}$$

by writing the propagator $\exp(-H\tau)$ as a product over short time intervals,

$$\exp(-H\tau)=\prod \exp(-H\Delta\tau)\ . \tag{2}$$

These short time propagators are then approximated as the product of a free particle propagator and an exponential factor involving the potential,

$$\exp(-H\Delta\tau)\approx\exp(-V\Delta\tau)\exp(-T\Delta\tau)\ . \tag{3}$$

This leads to errors in the propagator of order $\Delta\tau$ squared, which can be eliminated by performing calculations using different small values of $\Delta\tau$ and extrapolating to zero time step.

The integral equation for $\Psi(\mathbf{R},\tau)$ is

$$\Psi(\mathbf{R},\tau+\Delta\tau)=\int d\mathbf{R}'\exp[-V(\mathbf{R})\Delta\tau]\times N\exp\left[\frac{-(\mathbf{R}-\mathbf{R}')^2}{2\Delta\tau\hbar^2/m}\right]\Psi(\mathbf{R}',\tau)\ . \tag{4}$$

This integral equation is solved by using Monte Carlo methods to sample the free particle propagator and including branching to take the $\exp[-V(\mathbf{R})\Delta\tau]$ factor into account. The equation is then iterated until the system has converged.

In practice, Eq. (4) is multiplied by an importance function $\Psi^I(\mathbf{R})$ to improve the statistical accuracy of the method. This yields an equation:

$$\Psi^I(\mathbf{R})\Psi(\mathbf{R},\tau+\Delta\tau)=\int d\mathbf{R}'\Psi^I(\mathbf{R})\exp[-V(\mathbf{R})\Delta\tau]N\exp\left[\frac{-(\mathbf{R}-\mathbf{R}')^2}{2\Delta\tau\hbar^2/m}\right]\frac{1}{\Psi^I(\mathbf{R}')}\Psi^I(\mathbf{R}')\Psi(\mathbf{R}',\tau)\ . \tag{5}$$

When sampling from the Green's function with importance sampling, the ratio $\Psi^I(\mathbf{R})/\Psi^I(\mathbf{R}')$ is approximated with an expression accurate to first order in $\mathbf{R}-\mathbf{R}'$. After sampling $\mathbf{R}$, the result is corrected by introducing a weight given by $\Psi^I(\mathbf{R})/\Psi^I(\mathbf{R}')$ divided by the approximate value used to generate $\mathbf{R}$. This weight is multiplied by $\exp[-V(\mathbf{R})\Delta\tau]$ and used to control the branching of the population.

In principle, the extension of this method to treat spin-dependent interactions is straightforward. The Green's function then becomes an operator in spin space, again given to first order in $\Delta\tau$ by

$$\langle\mathbf{R},s\mid\exp(-H\Delta\tau)\mid\mathbf{R}',s'\rangle\approx\langle\mathbf{R},s\mid\exp(-V\Delta\tau)\mid\mathbf{R},s'\rangle N\exp\left[\frac{-(\mathbf{R}-\mathbf{R}')^2}{2\Delta\tau\hbar^2/m}\right], \tag{6}$$

where s and s' indicate spin states. The exact and trial wave functions are column vectors in spin space, and the equivalent of Eq. (5) is

$$\Psi^I_s(\mathbf{R})\Psi_s(\mathbf{R},\tau+\Delta\tau)=\int d\mathbf{R}'\Psi^I_s(\mathbf{R})\langle s\mid\exp[-V(\mathbf{R})\Delta\tau]\mid s'\rangle N\exp\left[\frac{-(\mathbf{R}-\mathbf{R}')^2}{2\Delta\tau\hbar^2/m}\right]\frac{1}{\Psi^I_{s'}(\mathbf{R}')}\Psi^I_{s'}(\mathbf{R}')\Psi_{s'}(\mathbf{R}',\tau)\ . \tag{7}$$

Two points must be addressed to perform a calculation. First, the exponential of $-V\Delta\tau$ must be calculated. For a system with more than a very few channels, computing the eigenvectors and eigenvalues of the potential matrix is impractical. Since $\Delta\tau$ must be small, the exponential must be evaluated a very large number of times to ensure convergence to the ground state. However, the evaluation of $\exp[-V(\mathbf{R})\Delta\tau]$ is only required to be accurate to first order in $\Delta\tau$. One could, of course, approximate the exponential by

$$\langle s\mid\exp[-V(\mathbf{R})\Delta\tau]\mid s'\rangle\approx\langle s\mid s'\rangle-\Delta\tau\langle s\mid V(\mathbf{R})\mid s'\rangle\ . \tag{8}$$

However, this would require an extremely small time step to give an accurate representation of the Green's function. The choice of approximation must be guided by the interaction itself. This point will be discussed in greater detail for the special case of the nucleon-nucleon interaction.

Assuming that an appropriate approximation to the short time Green's function can be obtained, the iteration of Eq. (7) is very simple. In order to propagate a configuration from one generation to the next, one must first divide the weight in each channel by the importance function in that channel. A new point $\mathbf{R}$ is chosen by sampling the free particle propagator, and the column vector representing the wave function is multiplied by the exponential of the potential matrix. Finally, the overlap in each channel of this column vector with the importance function at the new point is computed.

In general, the weights in each channel will not be real. However, one can use the real part of the sum of these weights to control the branching of the population, and determine the energy of computing the overlap of the exact wave function with a trial function Ψ^T.

$$E=\frac{\mathcal{R}\langle\Psi^T\mid H\mid\Psi\rangle}{\mathcal{R}\langle\Psi^T\mid\Psi\rangle}\ . \tag{9}$$

In principle the trial and importance functions may be different, but in practice they are often taken to be the same. As long as all regions of spin and coordinate space are accessible to the random walk, no approximations (except for the finite time step) need be introduced.

However, the statistical error of the calculation may grow for larger τ. The GFMC method will converge to the lowest eigenstate of the Hamiltonian consistent with

the spin symmetry properties of H. That is, if the Hamiltonian commutes with the total spin S, then the ground state determined by the GFMC method is the ground state of the system with the same spin as the trial wave function. As long as the approximation of $\exp[-V(\mathbf{R})\Delta\tau]$ preserves the same spin symmetries, the fact that all spin states are assumed over at each point in the walk ensures that states of different total spin will not enter.

However, the GFMC ground state may not be the physical ground state of the system. In this case, the Monte Carlo iteration of Eq. (4) will eventually converge to an unphysical state, giving a rapid increase in the statistical error.

The second source of increasing statistical error is present even if the GFMC ground state corresponds to the physical ground state. In this case, the sampling over paths introduces an arbitrary overall phase for each configuration. The difference between these phases grows for large τ, causing an increase in statistical error. However, in many cases (including light nuclei) this increase is slow enough to allow the true ground state to be accurately determined.

The wave function need not be positive definite in all channels in order for the GFMC method to succeed. For example, consider a one body problem in three dimensions. The diagonal elements of the potential are harmonic oscillators, and they are coupled by a term proportional to the third coordinate of the particle:

$$V=\begin{bmatrix} r^2 & z \\ z & 1+r^2 \end{bmatrix}, \tag{10}$$

with units given by $\hbar^2/2m=1$.

The ground state wave function of this system is spatially symmetric in the first channel, and spatially antisymmetric in the second, due to the odd parity coupling. Obviously, the wave function in the second channel is not positive definite. However, the GFMC method is stable over propagation times τ large compared to the inverse of the lowest excitation energy of the Hamiltonian. Assume an importance function that has the wrong sign in the second channel relative to the first, and that also has an incorrect spatial dependence,

$$\Psi^I=\begin{bmatrix} \exp(-r^2/2) \\ 0.4z\exp(-r^2/2) \end{bmatrix}. \tag{11}$$

The initial set of configurations give a distribution of weights in the two channels as shown in Fig. 1. At $\tau=0$ the weights are positive in both channels in all regions of configuration space since they are proportional to the square of the importance function in that channel. For larger τ, the weights in the two channels change as shown, eventually stabilizing at the ground state. Since the relative signs of the two channels are opposite for the exact and importance functions, the weights in the second channel eventually become negative. The energy, which is the overlap of $\langle \Psi^T \mid H \mid \Psi \rangle$, is shown as a function of τ in Table I.

The GFMC calculation is stable because components of the wave function with an incorrect relative sign decay more quickly than those with the relative sign of the ground state. This wave function is at least superficially similar to s-shell nuclei in that it consists of large spatially symmetric components of the wave function coupled to small negative parity components.

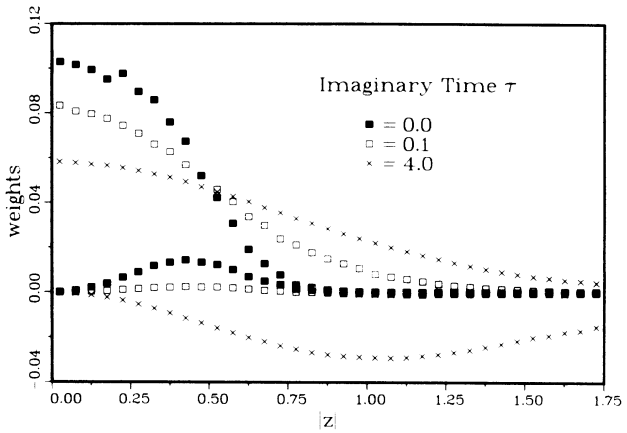

FIG. 1. Weights at different propagation times τ for the coupled harmonic oscillator problem in the text. The upper curves give the weights in the first channel, and the lower curves the weight in the second. The second channel has been multiplied by a scale factor for clarity.

For many problems the physical ground state of the system will not be equivalent to the GFMC ground state. In this case, it will sometimes be possible to use transient estimation techniques to project out the state of correct symmetry before the onset of large statistical error. In other cases, it will prove useful to introduce an approximation analogous to the fixed node method.

The fixed phase approximation is obtained by writing a wave function of the form

$$\Psi=\sum_{n=1}^{N} A_n(\mathbf{R}) \sum_{s=1}^{S} \phi_{ns}(\mathbf{R}) . \tag{12}$$

S is the total number of spin channels in the problem. In the fixed phase approximation, the number of channels may be reduced to any number N less than or equal to S. The spin states s are assumed to be orthonormal, as are the restricted basis states labeled by n. Constraints are placed upon the amplitudes $A_n(\mathbf{R})$ and the "phases" $\phi_{ns}(\mathbf{R})$. First,

$$\sum_{s,s'} \langle \phi_{ns}(\mathbf{R}) \mid \phi_{n',s'}(\mathbf{R}) \rangle = \delta_{n,n'} \tag{13}$$

for all values of $\mathbf{R}$, and the amplitudes A are real,

TABLE I. Coupled harmonic oscillators.

τ	Energy	Weight (1)	Weight (2)
0.0	3.101±0.005	0.990	+0.001
0.1	3.044±0.006	1.022	−0.022
0.2	2.972±0.006	1.039	−0.039
4.0	2.830±0.009	1.075	−0.075
Exact	2.829		

$$\mathcal{J}A_n(\mathbf{R})=0\ . \tag{14}$$

For a prescribed set of phases, one may then solve for the amplitudes which give the lowest variational energy. Writing out the expectation value of the Hamiltonian with this form of wave function and making use of the fact that H is Hermitian and A is real, the energy is

$$\begin{aligned}E=&\int d\mathbf{R}\sum_n A_n(\mathbf{R})\frac{-\hbar^2}{2m}\nabla^2 A_n(\mathbf{R})\\&+\int d\mathbf{R}\sum_{n,s} A_n(\mathbf{R})\frac{\hbar^2}{2m}[\nabla\phi^\dagger_{n,s}\cdot\nabla\phi_{n,s}]A_n(\mathbf{R})\\&+\int d\mathbf{R}\sum_{n,n',s,s'} A_{n'}(\mathbf{R})\tfrac{1}{2}(\phi^\dagger_{n,s}V_{s,s'}\phi_{n',s'}\\&\qquad+\phi^\dagger_{n',s'}V_{s',s}\phi_{n,s})A_n(\mathbf{R}).\end{aligned} \tag{15}$$

Therefore, the amplitudes A solve a Schrödinger equation with a Hamiltonian given by

$$H=\frac{-\hbar^2}{2m}\nabla^2+\tilde{V}_{n,n'}\ , \tag{16}$$

where the potential $\tilde{V}$ is

$$\begin{aligned}\tilde{V}_{n,n'}=&\sum_s\frac{\hbar^2}{2m}[\nabla\phi^\dagger_{n,s}\cdot\nabla\phi_{n,s}]\delta_{n,n'}\\&+\sum_{s,s'}\tfrac{1}{2}(\phi^\dagger_{n,s}V_{s,s'}\phi_{n',s'}+\phi^\dagger_{n',s'}V_{s',s}\phi_{n,s})\ .\end{aligned} \tag{17}$$

The first term in $\tilde{V}$ is associated with the kinetic energy of the phases, and the second term is the spin averaged potential. Any variational wave function may be written in the form of Eq. (12), and any wave function with an exact set of phases will yield the exact ground state energy.

The most drastic fixed phase approximation involves turning the problem into an equivalent one channel problem, and the least restrictive corresponds to fixing the complex phase of the wave function in each channel. In general, one would like to allow the most general wave function possible. The degree of approximation which must be made to retain stability depends upon the problem.

In one channel, this method is equivalent to writing $\Psi(\mathbf{R})=A(\mathbf{R})\exp[i\Theta(\mathbf{R})]$, requiring A and Θ to be real, and solving the equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2+\frac{\hbar^2}{2m}\,|\,\nabla\Theta\,|^2+V\right]A(\mathbf{R})=EA(\mathbf{R})\ . \tag{18}$$

The fixed node approximation is obtained by taking $\Theta=0$ where the trial wave function is positive, and $\Theta=\pi$ where it is negative. The "phase potential" is then zero except at the nodes, where it is represented by the square of a delta function, implying that no configuration may diffuse from the positive to negative regions of the trial wave function.

Approximations along these lines may also be valuable in scattering calculations. In the next section we discuss the applicability of these methods to light nuclei.

III. LIGHT NUCLEI

Models of nuclei as systems of interacting nucleons involve Hamiltonians of the form

$$H=\frac{-\hbar^2}{2m}\nabla^2+\sum_{i<j}\sum_k V^k(\,|\,\mathbf{r}_i-\mathbf{r}_j\,|\,)O^k_{i,j}\ , \tag{19}$$

where V^k are functions of the pair separation and the operators $O^k_{i,j}$ are, for example,

$$\begin{aligned}O^k=&1,\ \sigma\cdot\sigma,\ \tau\cdot\tau,\ \sigma\cdot\sigma\,\tau\cdot\tau,\ S,\ S\tau\cdot\tau,\ L\cdot S,\ L\cdot S\tau\cdot\tau,\ L^2\ ,\\&L^2\sigma\cdot\sigma,\ L^2\tau\cdot\tau,\ L^2\sigma\cdot\sigma\,\tau\cdot\tau\ .\end{aligned} \tag{20}$$

For this initial study, we consider two simplified Hamiltonians where only the first two and the first six operators are included, respectively. The ATS-3 (Ref. 19) interaction incorporates a difference between spin singlet and spin triplet channels, but no tensor or more complicated operator dependence. Its principle advantage for these calculations is that it has a relatively weak central core, approximately 1000 MeV, so it is feasible to use relatively large time steps and efficiently explore the possibilities of the method.

Results are also presented for a somewhat more complicated $V6$ interaction. The radial forms of the potential are taken to be those of the Argonne $V14$ (Ref. 21) interaction. The potential is truncated to these first six operators. Obviously this interaction will not correctly describe the scattering data, and it gives too small a binding energy for the deuteron. Nevertheless, it should provide a good test for variational calculations of the alpha particle.

The variational wave functions for the light nuclei are taken to be of the form

$$\Psi=\mathcal{S}\left[\prod_{i<j}F_{i,j}\right]\mathcal{A}\Phi\ . \tag{21}$$

The Φ are antisymmetric spin-isospin states of the correct spin and isospin for the nucleus of interest. The pair correlation operators $F_{i,j}$ involve spin and isospin operators and are determined by solving two body differential equations. References 13 and 14 give somewhat different asymptotic boundary conditions on the pair correlations. The second set of boundary conditions (Ref. 14) give more accurate asymptotic normalizations, but for the alpha particle no statistically significant improvement in the binding energy is obtained. Both sets of boundary conditions have been employed in the GFMC calculations. The Metropolis Monte Carlo procedure used to determine the variational energy is described in Ref. 12.

An approximation to $\exp[-V(\mathbf{R})\Delta\tau]$ must be developed for GFMC calculations of light nuclei. For the alpha particle, a brute force diagonalization would be just feasible even on a supercomputer, as a crude estimate indicates that several hundred central-processing-unit (CPU) hours on a Cray XMP would be required.

It is apparent that an approximation to $\exp[-V(\mathbf{R})\Delta\tau]$ is required. Whatever approximation is chosen, it must be accurate to at least first order in $\Delta\tau$, and should provide a good approximation to the com-

plete exponential when two particles are near each other. In addition, efficient calculations of the approximation must be feasible.

We have chosen to approximate the exponential by

$$\exp[-V(\mathbf{R})\Delta\tau] \approx \mathcal{S}\left[\prod_{i<j}\exp(-V_{ij}\Delta\tau)\right] . \quad (22)$$

The $\mathcal{S}$ stands for a symmetrization operator, indicating in this case a random choice of the order of pairs in the product. This form is accurate to first order in $\Delta\tau$, and it also closely approximates the full exponential in the core region. Errors of higher order in $\Delta\tau$ arise only due to the fact that the potential operators from different pairs do not commute. These errors are large only when three or more particles overlap within a core region, a very restricted part of phase space.

In addition, this approximation to the exponential may be calculated very efficiently. Consider the potential written in the spin-isospin channel representation:

$$V = \begin{cases} V_{00}(r), & S=0, \quad T=0 \\ V_{01}(r), & S=0, \quad T=1 \\ V_{10}(r)+V_{t0}(r)S_{ij}, & S=1, \quad T=0 \\ V_{11}(r)+V_{t1}(r)S_{ij}, & S=1, \quad T=1 \ . \end{cases} \quad (23)$$

The spin singlet channels are not coupled to the spin triplet, and the isospin zero and isospin one channels are also not coupled to each other. Therefore, in the spin singlet channels, the exponential of the potential carriers no operator dependence. In the spin triplet channels, it is possible to rewrite the potential as

$$V = \begin{cases} \bar{V}_{10}(r)+\bar{V}_{t0}(r)\bar{S}_{ij}, & S=1, \quad T=0 \\ \bar{V}_{11}(r)+\bar{V}_{t1}(r)\bar{S}_{ij}, & S=1, \quad T=1 \end{cases} \quad (24)$$

where the operator $\bar{S}_{ij}$ is given by

$$\bar{S}_{ij} = \sigma_i \cdot \hat{r}_{ij} \sigma_j \cdot \hat{r}_{ij} \ . \quad (25)$$

Since $(\bar{S}_{ij})^2 = 1$, the exponential in these channels is

$$\exp(-V\Delta\tau) = \exp(-\bar{V}\Delta\tau)[\cosh(-\bar{V}_t\Delta\tau) + \sinh(-\bar{V}_t\Delta\tau)\bar{S}_{ij}] \ . \quad (26)$$

Once the exponential is calculated in channel form, it may easily be converted into operator form to calculate $\exp(-V(\mathbf{R})\Delta\tau)$ acting on the wave function.

For the alpha particle, the Coulomb interaction is taken from Ref. 14. It includes a cutoff from the charge distribution of the protons. The projection onto a $T=0$ trial wave function introduces an extremely small error, much smaller than the statistical error of the calculation.

IV. RESULTS

We first review the results of the triton calculations with the ATS-3 interaction. This interaction incorporates only different spin singlet and spin triplet interactions. The results of several different calculations are presented in Table II. The asymptotic form of the variational wave function was taken from Ref. 13. The parametrization of Ref. 14 yields somewhat better binding energies and asymptotic normalizations for the three nucleon system, but we are primarily interested in testing the GFMC method.

The variational wave function, which was not carefully optimized, yields a binding energy of -8.12 ± 0.03 MeV for the triton. Faddeev methods[22] give a binding energy of -8.765 MeV, for a difference of approximately 0.65 MeV.

The first GFMC calculation was a fixed phase approximation restricted to only one channel. With a relatively small time step (2.0×10^{-4} MeV^{-1}), the binding energy was almost identical to that of the variational calculation. This fixed phase approximation solves for the lowest energy state with the same relative magnitude in all spin channels as the variational wave function. The fact that the GFMC energy is very near the variational energy (and quite different from the Faddeev) indicates that the deficiencies of the variational wave function are embedded in its spin dependence. This result is consistent with many calculations of spin-independent interactions for $A=3$ and 4 nuclei, for which variational, GFMC, and Faddeev calculations agree very well.

The other calculations listed in Table II do not involve a fixed phase approximation. Two different time steps were used, and the configurations were propagated for a total time of 0.7–1.0 MeV^{-1}. This time is more than enough to ensure convergence to the ground state, since the first fermion excited state is at approximately 5 MeV. During these calculations, the weights of a very few (approximately 0.5%) of the configurations became negative. The contributions of these walks were retained in the averages given in the table. Eventually these negative weights would lead to large statistical errors, but only long after convergence to the ground state.

In all cases, a linear extrapolation has been used to determine the zero time step result. Although the error

TABLE II. Triton with ATS-3 interaction.

Method	Time step (MeV^{-1})	Energy (MeV)	$\langle V_{ij}\rangle$ (MeV)	$\langle r_i^2\rangle^{1/2}$ (fm)
Variational		-8.12 ± 0.03	-40.0 ± 1.0	1.68 ± 0.03
Faddeev (34 channels)		-8.76		
Fixed phase GFMC	2.0×10^{-4}	-8.15 ± 0.02	-40.6 ± 1.0	1.66 ± 0.04
GFMC	1.0×10^{-3}	-8.87 ± 0.04	-43.9 ± 0.9	1.66 ± 0.04
GFMC	5.0×10^{-4}	-8.80 ± 0.07	-42.4 ± 1.0	1.69 ± 0.05
Extrapolation		-8.73 ± 0.10	-40.9 ± 1.5	1.72 ± 0.07

TABLE III. Triton with $AV6$ interaction.

Method	Time Step (MeV^{-1})	Energy (MeV)	$\langle V_{ij} \rangle$ (MeV)	$\langle r_i^2 \rangle^{1/2}$ (fm)
Variational		-6.33 ± 0.05	-43.7 ± 1.0	1.95 ± 0.03
Faddeev (5 channels)		-6.46		
Faddeev (34 channels)		-7.15		
GFMC	4.0×10^{-4}	-7.23 ± 0.08	-49 ± 1	1.88 ± 0.04
GFMC	2.0×10^{-4}	-7.20 ± 0.08	-50 ± 1	1.83 ± 0.03
GFMC	1.0×10^{-4}	-7.23 ± 0.08	-49 ± 1	1.85 ± 0.03
Extrapolation		-7.22 ± 0.12	-52 ± 3	1.75 ± 0.10

in the Green's function is second order in $\Delta\tau$, the number of steps required for a given total propagation time is of order $\Delta\tau^{-1}$. More thorough checks of the extrapolation would be useful, but the extrapolations are generally quite small. For the ATS-3 interaction, the extrapolation of the GFMC calculations agrees with the Faddeev results within the statistical error of approximately 0.15 MeV.

The next set of calculations are for the triton with the "Argonne $V6$" interaction. In this case, the asymptotic boundary conditions on the variational wave function were taken to have the more accurate forms of Ref. 14. However, the precise values of the variational parameters were not carefully optimized. The variational binding energy obtained was -6.33 ± 0.05 MeV. The 34 channel Faddeev result for this same interaction is -7.15 MeV.[22] This difference between variational and Faddeev results is significantly larger than for more realistic potentials, so great care must be used when trying to draw parallels between calculations using different interactions. Faddeev calculations restricted to only five channels also give a small binding, as listed in Table III. Thus, the effects of the higher partial waves appear to be more important than for more realistic potentials.

GFMC results are listed for three different time steps. Each calculation employed approximately 4000 configurations which were propagated for a total imaginary time of 0.4 MeV^{-1}. The results given in Table II were obtained by averaging between $\tau=0.2$ and $\tau=0.4$ MeV^{-1}.

The convergence of the calculation to the true ground state energy can be determined by examining the energy as a function of τ. Since the first excited state of the trinucleon system is at approximately 5 MeV, the contribution of even the lowest excited state decreases by a factor of $1/e$ in a time of 0.2 MeV^{-1}. By comparing the average between 0.01 and 0.20 MeV^{-1} to that between 0.2 and 0.4, the energy can be shown to have converged to within several hundredths of a MeV, much less than the statistical errors of the calculations.

It is possible to accurately calculate the ground state of the triton because the lowest state of the system is the antisymmetric one.[23] These calculations could be extended to a somewhat larger τ without a great increase in statistical error. However, the statistical error will eventually increase because of the arbitrary relative phase introduced in the Monte Carlo sampling.

Extrapolation of the GFMC results to zero time step gives a binding energy of 7.22 MeV, which is again consistent with the Faddeev result. The statistical error of the calculation is approximately 0.12 MeV. The expectation values of the Argonne $V6$ interaction and the point nucleon radii are also given in Table II. The result for quantities other than the ground state energy is determined by first extrapolating to zero time step, and then extrapolating from that mixed estimate to the ground state expectation value.

Finally, ground state properties of the alpha particle were calculated. For the alpha particle, no other exact method is presently available. Variational wave functions with the asymptotic boundary conditions of both Refs. 13 and 14 were employed, and the optimum values of the variational parameters obtained for each case. The energy of the two variational forms were statistically indistinguishable, but the statistical error associated with the first form seemed to be slightly lower than that of the second. Consequently, it was chosen as the trial wave function for the GFMC calculations.

The results of the alpha particle calculations are summarized in Table IV. In this case approximately 2000 configurations were employed, and they were propagated for a total imaginary time of 0.15 MeV^{-1}. The first excited state of the alpha particle is at approximately 20 MeV excitation energy, so that the system should have converged to the ground state. As for the triton, the GFMC energy stabilized very quickly, and no statistically significant decrease in energy occurred after a propagation time of approximately 0.03 MeV^{-1}.

TABLE IV. Alpha particle with $AV6$ interaction.

Method	Time Step (MeV^{-1})	Energy (MeV)	$\langle V_{ij} \rangle$ (MeV)	$\langle r_i^2 \rangle^{1/2}$ (fm)
Variational		-22.75 ± 0.10	-122 ± 1	1.50 ± 0.01
GFMC	1.0×10^{-4}	-24.89 ± 0.12	-126 ± 1	1.49 ± 0.02
GFMC	5.0×10^{-5}	-24.84 ± 0.09	-124 ± 2	1.50 ± 0.02
Extrapolation		-24.79 ± 0.20	-122 ± 30	1.50 ± 0.04

Two different values of the time step were used. These values are smaller than those used for the triton since the system is more dense and the potential energy is larger by roughly a factor of 2. Extrapolating to zero time step, a ground state energy of -24.8 MeV is obtained, with a statistical error of approximately 0.2 MeV. Thus, the GFMC ground state energy lies approximately 2 MeV below the variational energy.

The population growth can also be used to estimate the ground state energy. This estimate of the energy is below the variational result and consistent with the GFMC mixed estimate result, but has a somewhat higher error bar and a larger time step dependence.

The increase in binding energy obtained with GFMC methods is not large enough to explain the difference between experiment and variational calculations with two nucleon interactions alone. Models of the two pion exchange three nucleon attraction therefore remain attractive candidates for understanding the binding energy of the alpha particle.

On the other hand, it appears to be premature to draw conclusions about details of the three nucleon interaction from variational results. GFMC studies with more realistic interactions seem likely to given an energy 1–2 MeV lower than variational calculations. Methods to incorporate more accurate interaction models are being investigated, and the possibilities are described briefly in the next section.

In addition to the binding energy, the point nucleon distribution function of the alpha particle has also been computed with both the variational and GFMC methods. The results are presented in Fig. 2, where the curve labeled "GFMC" gives the mixed estimate for the one body distribution function. This estimate is obtained by taking the overlap of the variational and GFMC wave functions. No extrapolation to the exact distribution function has been attempted, since the statistical errors of each curve are comparable to the differences between them.

The GFMC one body distribution has less structure for $r < 0.5$ fm than the variational curve. In general, it appears that form factors obtained from variational calculations should be fairly accurate at low momentum transfer, but may be in error for larger values of q^2.

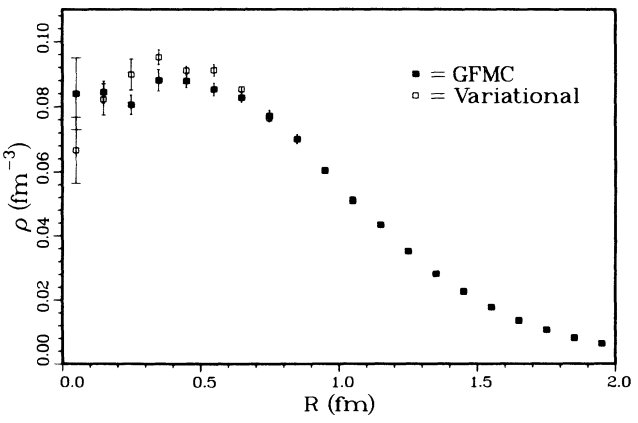

FIG. 2. Point nucleon distribution for the alpha particle with the $AV6$ interaction. The curve labeled "GFMC" is the mixed estimate for the smallest time step used (see text).

The spin-isospin averaged pair distribution function has also been calculated with both methods. This distribution is proportional to the probability of finding two nucleons separated by a distance r, averaged over all of the spin and isospin states of the pair. The pair distributions of the two calculations are nearly identical.

The difference between variational and GFMC binding energies of the alpha particle is slightly more than twice as large as in the triton. This suggests that the two body correlations may not be sufficiently accurate in the variational wave function. In this regard, it may prove instructive to compare the pair distribution functions in the four spin-isospin channels.

V. SUMMARY AND OUTLOOK

The calculations and methods presented in this paper demonstrate the practicality of GFMC calculations for systems with spin-dependent interactions. The methods should prove to be very valuable in many areas of nuclear physics. The applications to light nuclei are obvious. In addition, GFMC methods should allow accurate ground state calculations to be performed for many quark models. Constituent quark models of single- or few-hadron systems typically involve a Hamiltonian with a strong spin dependence, usually modeled as a one gluon exchange[24] interaction. GFMC methods should be applicable to many of these problems. Nonrelativistic models[25,26] may be calculated exactly as described, while "semirelativistic" models[27] [which use a $(p^2+m^2)^{1/2}$ kinetic energy operators] involve only the introduction of a different free particle propagator. Quark models are presently being studied with GFMC methods.

These calculations demonstrate that great care must be taken when trying to draw conclusions from relatively fine details of variational calculations of the alpha particle. For the triton, this $V6$ interaction yields an unusually large difference between variational and Faddeev results. Variational calculations of the alpha particle with more realistic interactions may also be more accurate than for this $V6$ interaction. However, this $V6$ model significantly underbinds helium-4, and the larger central density associated with more realistic two and three nucleon interactions may increase the error in the variational calculations.

There is an obvious need for extensions of GFMC methods to more complicated interactions involving momentum dependent terms and three nucleon interactions. These terms are relatively small for nuclear interactions, and it may be feasible to keep only first order terms in $\Delta\tau$, and still retain a low statistical error. Three nucleon interactions are simple to treat in this way, since it is only necessary to calculate the interaction acting on the wave function. Momentum dependence is more difficult to handle, but may still be feasible to first order in $\Delta\tau$. The essential element in employing a momentum dependent interaction is to write down the integral equation for the wave function to first order in delta tau and use integration by parts to remove the

derivative operators. These calculations are being vigorously pursued.

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