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TITLE **Green's Function Monte Carlo Calculations of Light Nuclei**

AUTHOR(S) **J. Carlson**

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Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Green's Function Monte Carlo Calculations of Light Nuclei

J. Carlson

T-5, MS B283, Los Alamos National Laboratory, Los Alamos, NM 87545

Recently, Green's Function Monte Carlo methods have been developed which enable one to perform exact calculations for the ground states of three and four body nuclei. These methods allow the alpha particle to be used as a testing ground for a variety of two- and three-nucleon interaction models, both in terms of their ground state energies and a variety of other ground state expectation values.

We present a brief review of GFMC methods as applied to light nuclei, including recent improvements of the algorithm and a discussion of the prospects for the inclusion of momentum-dependent terms. We then discuss results for the ground state energy, one- and two-body density distributions, D state probability, coulomb sum rule, and momentum distributions. The GFMC results are compared to experimental results and to variational Monte Carlo calculations.

1. INTRODUCTION

Over the past two years, Green's function Monte Carlo (GFMC) methods have been developed[1,2] which allow one to perform exact calculations of the ground states of few body nuclei. GFMC and related methods[3-6] have proven to be very valuable in determining the ground state properties of few- and many- body quantum systems, including atomic and molecular systems[7,8] and quantum fluids and solids[9,10].

In the next section, we present a brief review of the algorithm, including a discussion of improvements to the basic algorithms described in references 1 and 2. The difficulties associated with the inclusion of momentum dependent terms in a GFMC algorithm are also discussed.

In [illegible] we present results for the Reid V8 and an Argonne V8 interaction model. The [illegible] in the four body system compared to variational results requires a significantly smaller three nucleon interaction to reproduce the experimental binding energies. We [illegible] results obtained to date for the momentum distribution, the charge form factor [illegible] coulomb sum rule [illegible] their implications.

2. GFMC

Green's function Monte Carlo and related methods attempt to project out the ground state [illegible] equation:

$$\Psi = \mathrm{Tr}\exp(-H\tau)\Psi_T$$

where Ψ_T is an initial trial state, typically obtained from a variational calculation. By dividing the propagation time τ into many small steps $\Delta\tau$,

$$\exp(-H\tau) = \prod_{i=1}^{n} \exp(-H\Delta\tau) = \int G(\vec{R}_i, \vec{R}_{i-1}) \cdots G(\vec{R}_1, \vec{R}_0) \qquad 2$$

one can evaluate the matrix elements for each short time propagator $G(\vec{R}', \vec{R})$. Monte Carlo is employed to perform the integrals over all coordinates at each intermediate time step.

For short propagation times $\Delta\tau$, the following approximation[11] is quite useful:

$$G(\vec{R}, \vec{R}') \approx G^0(\vec{R}, \vec{R}') \prod_{i=1}^{n} \frac{g_i(\vec{r}_i, \vec{r}'_i)}{g_i^0(\vec{r}_i, \vec{r}'_i)} \qquad 3$$

In this equation, the full G for 3A coordinates is approximately given by the free particle propagator, a gaussian, times a product of all pair propagators divided by their respective free particle propagators. The simplest approximation to the ratio in equation 3 is, of course

$$g(r, r') = \exp(-\Delta\tau/2)(V_i(r) + V_i(r')), \qquad 4$$

where V_i and consequently g_i are operators in spin isospin space. It is possible, and in fact very valuable in certain cases, to solve numerically for the full pair Green's function. Incorporating the two body solution is most important for the case of hard core potentials, a typical case being quantum liquids and solids.[11] Nuclear interactions, though, often have relatively soft cores, but involve the additional complexity of several spin and isospin channels. Solving and tabulating many six dimensional functions is a rather daunting task.

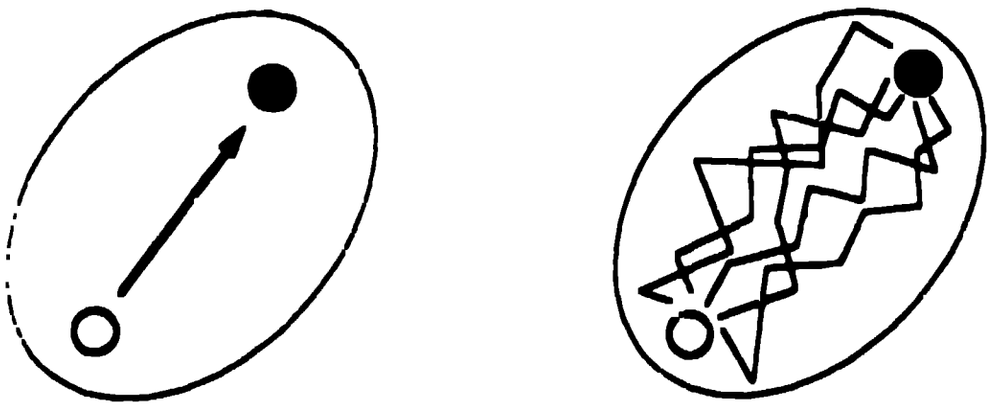

Figure 1. Sampling of internal paths to determine the pair propagator.

Fortunately, this is not necessary for nuclear problems, as we can sample a set of paths to determine the pair Green's function. The procedure is illustrated in figure 1. The left figure

represents the approximation given in equation 1, where we only compute the potential at the two end points. However, by further subdividing the path one can obtain a much better approximation to the pair Green's function. In the right hand figure, the path has been divided into several sub paths, each with a much shorter time step than the original walk.

Further, the antithetic sampling of the sub walks is quite useful. A simple example of this procedure would be to include a mirror image reflected about the pair axis of each path that is sampled. In this work, we typically divide a step into four paths, each of which is divided into eight smaller steps. The overall time step is limited by three body effects, etc., which are large due to the spin-isospin structure of the interaction. We typically take the overall time step to be of the order of 0.005 MeV^{-1}, yielding an effective pair time step of 0.25×10^{-4}, which should be more than sufficient for standard nuclear interactions.

It is very simple to exponentiate the potential for one pair, and thus to evaluate this more accurate expression for the Green's function. For this reason, the efficiency of the GFMC algorithm can be improved by a factor of 1.5 over the simplest equation 1 methods.

The preceding discussion of the GFMC algorithm assumes that the potential contains no momentum dependent terms. Realistic models of the NN interaction do contain such pieces, including $\vec{L}\cdot\vec{S}$, $\vec{L}^2$, $\vec{S}\cdot\vec{S}$, and p_θ^2 operators. Incorporating the most realistic Hamiltonians with all of these terms remains an outstanding problem, although some progress has been made. It is quite feasible to include $\vec{L}\cdot\vec{S}$ operators in the GFMC algorithm,[2] as they involve only the momentum operator. By simply evaluating the $\vec{L}\cdot\vec{S}$ acting on the free particle Green's function, one can obtain an expression for the full Green's function valid to [illegible] time step. The resulting full propagator is

$$G(\vec{R},\vec{R}') = \sum_{\alpha} \Lambda_\alpha(\vec{L}\cdot\vec{S}) \, G^0(\vec{R},\vec{R}') \cdot \prod_{i<j} g_{ij}(r_{ij}) \qquad (5)$$

[illegible] to be the derivative operator act only on the free particle Green's function [illegible] evaluate the pair Green's functions for the momentum independent interaction as [illegible] described.

The inclusion of higher order momentum dependent terms is much more difficult, however. In order to illustrate the difficulties, we consider a simple two body problem with only a [illegible] dependent $\vec{L}^2$ term. The Green's function in this case requires a different effective [illegible] in the angular coordinates. It is easy to construct an algorithm to sample this distribution. The essential ingredient is a step size in the direction orthogonal to r_{ij}, different from [illegible] along the radial direction (figure [illegible]). Central $\vec{L}^2$ terms for N body problems can also be treated [illegible]. It should be noted, though, that the different pair displacements are not independent. Therefore, the full Green's function cannot be written as a product of [illegible] as in equation 5.

For central momentum dependent operators, then, require different effective steps in each of the spin-isospin channels. It is easiest to accomplish this by sampling a [illegible] Green's function, and introducing weights to account for the different masses in [illegible]

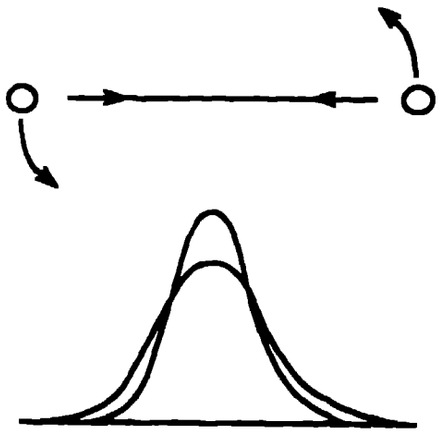

Figure 2. Effective masses in propagator for T^2 terms.

channels. The weights, though, no longer tend toward one as we decrease the time step. The ratio of two distributions with different rms radii are independent of the chosen time step.

The introduction of these large weights, in general, greatly reduces the stability of the method, and requires 'transient estimation' techniques commonly employed in many body fermion problems. Work is currently underway to try to develop the most efficient algorithms for these Hamiltonians. A large body of interesting physics can be attacked, though, with current techniques. In the following section we summarize the results obtained to date.

3. RESULTS

Since Faddeev methods[illegible] provide essentially exact results for the three nucleon system, GFMC is primarily of interest in treating nuclei with $A > 4$. We hope that GFMC will be practical for systems larger than the alpha particle and for excited states, yielding more accurate results than those obtainable from variational calculations. In this section we present alpha particle results for Reid V8 and Argonne V8 interaction models, which are simplifications of the full models in that they contain only T, S momentum dependent terms.

The variational and GFMC results for the alpha particle are summarized in Table 1, which includes the ground state energy, the expectation value of various terms in the interaction, the rms radii, and the D state percentage. The Argonne V8 model employed here is obtained by truncating the original AV14 model to eight operators and changing the $T = 0$, T, S term to give the correct interaction in the $^3D_1$ channel. It reproduces the deuteron, but the odd parity waves in this model give significantly more attraction than in the full Argonne V14. In the three body system, for example, it gives approximately 0.5 MeV more binding

in an eighteen channel Faddeev calculation.[15] We took the variational wave function for this interaction to be the same as that used for the full Argonne V14 optimized without any three-nucleon interaction (TNI).

Table 1. Alpha Particle Results

	Reid V8 Var	Reid V8 GFMC	AV8 Var	AV8 GFMC	AV14 Var
Energy	23.1(0.1)	24.6(0.2)	24.6(0.1)	26.5(0.2)	23.2(0.1)
KE	101.6(0.7)	109.2(2.0)	90.3(0.7)	101.1(2.0)	88.5(1.0)
V_0	127.6(0.7)	137.5(2.0)	113.3(0.5)	127.5(2.0)	111.6(0.9)
V_{LS}	2.2(0.1)	2.5(0.2)	2.3(0.1)	2.7(0.2)	1.2(0.1)
V_{τ}					12.6(0.2)
$V_{LS\tau}$					11.6(0.2)
$V_{\tau\tau}$	0.71(.01)	0.71(.02)	0.71(.01)	0.73(.02)	0.70(.01)
TNI_s			3.2(0.1)	3.7(0.2)	3.1(0.1)
$TNI_{2\pi}$			7.[illegible](0.1)	10.2(0.3)	7.0(0.2)
[illegible]	1.58(.01)	1.53(.01)	1.59(.01)	1.50(.02)	1.6[illegible](.01)
D^*	14.8(0.1)	15.5(0.2)	13.7(0.1)	15.0(0.2)	13.7(0.[illegible])

GFMC calculations for these two models give an increase in binding of 1.5 to 2 MeV compared to the variational results. Variational calculations with the most realistic two nucleon interactions underbind the alpha particle by approximately 5 out of the experimental 28.3 MeV; apparently about 1.5 MeV of this discrepancy can be traced to inadequate variational wave functions.

This error in the ground state energy is a significant fraction of the difference between variational and experimental results, but it is a very small fraction of the total kinetic or potential energies, which are each of the order of 100 MeV. Thus, the ground state energy results from a delicate cancellation between kinetic and potential terms, and it is very difficult for a variational wave function to reproduce this cancellation to a very high degree of accuracy.

The expectation values for the Urbana Model VII TNI[16] interaction are also indicated in Table 1. This model has been determined by fitting the binding energies of 3 and 4 body nuclei as obtained in variational calculations. Using the corrected ground state energies from Faddeev and GFMC calculations would reduce the strengths by roughly 20%. There does not appear to be sufficient freedom in this model, however, to reproduce both 3 and 4 body nuclei and the saturation properties of nuclear matter. Reducing the strengths gives a nearly correct saturation density, but too small a binding energy in nuclear matter calculations.[17]

Ground state expectation values other than the energy are extrapolated from variational and mixed estimates.

$$\Psi \rightarrow \Psi \qquad \Psi_T \rightarrow \Psi \qquad \Psi_T \rightarrow \Psi_T$$

This extrapolation is required because we are solving for Ψ rather than Ψ^2. This equation is only an approximation, but has often proven to be quite useful. More accurate calculations of the expectation values are possible, but very difficult to implement successfully. No extrapolation is necessary for the energy, of course, because the true wave function is an eigenstate of the Hamiltonian.

The primary differences between variational and GFMC calculations are, as one would expect, associated with the increased binding obtained in the exact calculation. GFMC gives a somewhat smaller rms radius for the nucleons, and also an increased magnitude for the potential and kinetic energies. In addition, the D-state probability is somewhat larger in the two cases presented here, causing a corresponding increase in the importance of the two-pion-exchange portion of the three nucleon interaction. It is quite feasible to include three-nucleon interactions in the GFMC algorithm (here they are treated perturbatively), and hence to determine the importance of the induced three body correlations in the alpha particle.

The momentum distribution of the nucleons has also been calculated with GFMC for the AV8 model. Although the curves in figure 3 are plotted on a logarithmic scale, it is clear that the variational calculations provide a good estimate of the momentum distribution, at least up to $\approx 1.5\ \mathrm{fm}^{-1}$. Beyond this point the statistical errors in the calculations are comparable to the value of the momentum distribution. The mixed estimate for the GFMC is plotted here, since the statistical errors in the two calculations are comparable to the differences between them. There are some differences between the two distributions, of course, since the kinetic energy (the second moment) differs by roughly 10%. There is also some difference at $k=0$, where the value of $n(k)$ depends strongly upon the radius of the system.

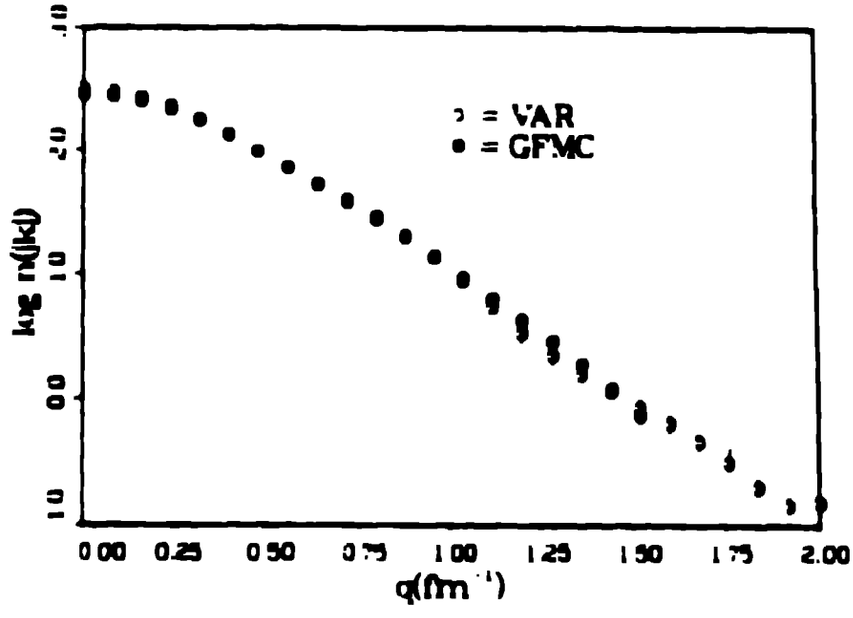

Figure 3. Momentum distributions in $A=4$

The charge form factor and coulomb sum rule of light nuclei are also important quantities of current interest. Results for the charge form factor, calculated in the impulse approximation, are presented in figure 4, along with the experimental values. At small momentum transfer, the difference between the two calculations is solely due to the decreased rms radius obtained with GFMC. The most important differences occur at larger values of q^2, near the region of the diffraction minimum and beyond. In the region of the second maximum, the variational results are much smaller than those obtained with GFMC. The form factor at large momentum transfer involves a delicate cancellation between the inner and outer portions of the charge density, so it is not too surprising to find significant differences in these calculations. Neither calculation includes any effects of exchange currents, so neither curve approaches the experimental results in the region of the second maximum.

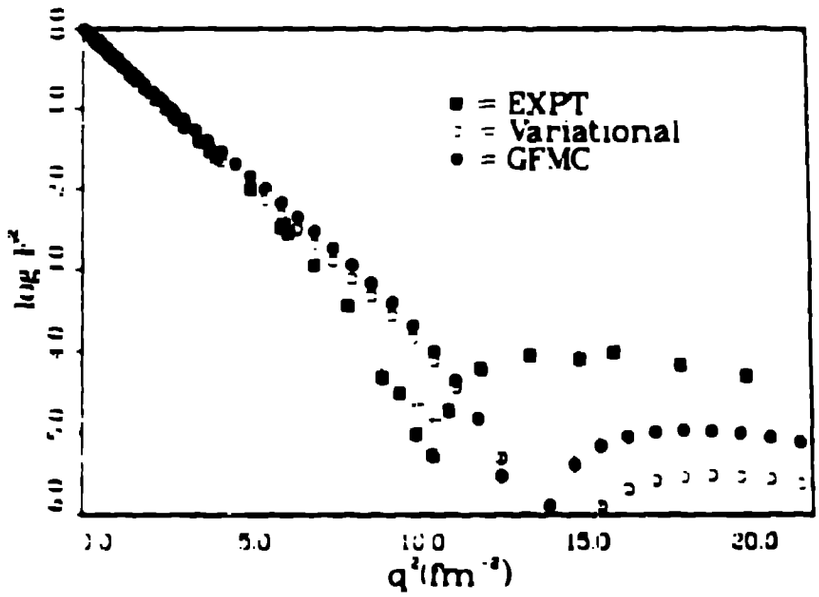

Figure 4 Charge form factor of the alpha particle, AV8 model

The longitudinal response of light nuclei has been the subject of a great deal of current experimental interest.[18,19] We have calculated the coulomb sum rule with the Argonne V8 interaction model, the results are shown in figure 5. The longitudinal structure function can be calculated as a ground state expectation value, it can be written approximately as:

$$S_L(q) \approx 1 - \rho_{pp}(q) + Z^2 F_\alpha(q)|^2 \qquad (7)$$

There are small additional contributions from the neutrons, which have been included in the calculations, but are not important for the purposes of this discussion. The experimental data are shown as open symbols in the figure, the experiments involve a cut off in ω, and therefore do not exhaust the sum rule. R. Schiavilla et al.[20,21] have calculated the ω and ω^2 sum rules from variational wave functions, and used these values to estimate the response above the experimental ω_{max}. The results of this extrapolation are indicated by solid points

in the figure. It will be interesting to see if GFMC calculations of the energy-weighted sum rule lead to any differences in the extrapolation

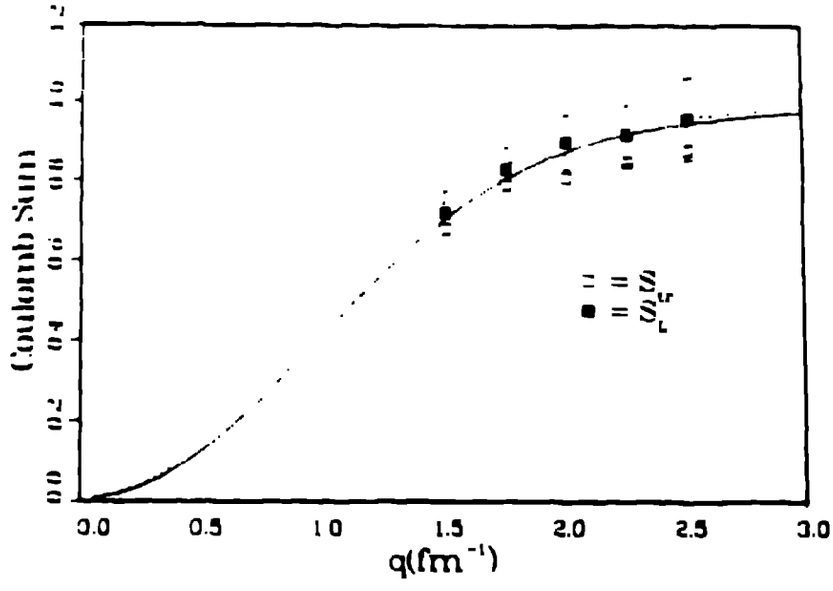

Figure 5: Alpha Particle Coulomb Sum, AV8 model

The upper (dotted) line is the 'uncorrelated' structure function, given by

$$S_{uc} = 1 - F_{ch}^2(q). \tag{8}$$

This represents the expected coulomb sum if there were no correlations between the two protons. Here it is calculated from the variational charge form factor.

The middle (dashed) curve shows the full coulomb sum obtained with the variational wave function. There is a significant depression associated with the repulsive core of the NN interaction. The solid curve gives the GFMC results which show a somewhat larger depression. The experimental limitations at this point are too great to distinguish between these two curves, they must be done more accurately and extended to higher energy in order to sort out such detail. Even this difference, though, appears to largely be a result of the different charge radii obtained in the two calculations, as opposed to any large differences in the correlations between the protons. Indeed, the pair distribution of protons in the nucleus are almost identical in the two sets of calculations.

4 CONCLUSION

Green's Function Monte Carlo can provide exact results for the ground state of A = 4 nuclei. The inclusion of more realistic models of the nuclear interaction remains an outstanding problem in these calculations, however. Significant improvements to the current algorithm will be necessary to treat momentum dependent terms. Nevertheless, a variety of interesting physical questions remain which can be addressed with somewhat simpler models.

In particular, it will be interesting to study the non-perturbative effects of the three nucleon-interaction. They may be more important here than in the A=3 system, because the density of the nucleus is larger and there are four triplets instead of one. It will also be important to look more closely at the electromagnetic response of these nuclei, in particular the inclusion of exchange current effects.

Over a somewhat longer term, two important problems should be addressed. First, larger systems (light p-shell nuclei) are important because they will provide more stringent tests of the interaction models in negative-parity channels. In addition, by studying nuclei such as ^{6}He, ^{6}Li and ^{8}Li, it may be possible to obtain much greater insight into the isospin dependence of the three nucleon interaction, which is important for neutron stars.

It is also important to see how well the interaction models do in predicting low energy scattering properties of few-nucleon systems. Properties of these states can be determined by converting the problem of determining the boundary condition at a specific energy to an eigenvalue problem with a given boundary condition.[22,27] Variational Monte Carlo calculations have shown that such calculations are feasible, but they generally miss the positions of the resonances by 1-2 MeV. These calculations suffer from the fact that it is uncertain whether the variational ansatz made for the scattering wave function is adequate, but GFMC may be able to overcome this problem.

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