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Variational Monte Carlo calculation of ^{16}O

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Many microscopic studies of both nuclear matter and s-shell nuclei have been undertaken with recently developed realistic models of the nucleon-nucleon interaction. These studies have proven to be very useful in enhancing our understanding of nuclear structure. Microscopic treatment of all but these lightest nuclei ($A<5$) has proven to be extraordinarily difficult, however, because of the strong spin-isospin dependence of the interaction. We have developed a new method of performing variational calculations with realistic interactions for larger nuclei. This method does not rely upon spin and spatial symmetries of the system, as in nuclear matter calculations, or upon explicit summation over all spin states, as has been done in s-shell nuclei. Instead spin-isospin states are sampled in a random walk which takes place in a combination of spin, isospin, and coordinate space. Results of calculations of the oxygen nucleus with a V6 interaction are reported, including energy, form factor, and charge distribution.

I. INTRODUCTION

In recent years, several realistic models of the nuclear interaction have been introduced.[1–3] These interactions have been employed in variational calculations of nuclear matter[4,5] and light nuclei,[6–8] and have resulted in many useful insights into areas such as three-nucleon interactions,[7–9] exchange currents,[10] etc. However, these microscopic studies have been limited in the sense that many facets of nuclear structure, such as surface effects, Coulomb energy, and excited states, have been studied in only a few special cases.

It is not feasible to directly apply the methods used for light nuclei or nuclear matter to heavier nuclei. For light nuclei, variational Monte Carlo[6–8] and Faddeev[11] techniques have been employed. The variational Monte Carlo method used in these systems entails a complete summation over all spin and isospin states of the system. There are $2^A A!/[Z!(A-Z)!]$ such states for a nucleus of A nucleons with Z protons, so the summation is possible only for very light nuclei. On the other hand, integral equation techniques have been used in studies of nuclear matter with many different interactions. These techniques rely to a great extent upon the spatial and spin symmetries of the system; symmetries that are not present in finite nuclei.

Consequently, microscopic studies of these larger systems have been limited to shell model[12] and coupled cluster[13] techniques. The ultimate aim of our work is to enable accurate variational calculations to be performed for much larger nuclei. The attainment of this goal would provide the possibility of studies in many areas previously inaccessible to microscopic calculations.

Our initial calculations have been performed on the ^{16}O nucleus, with a V6 interaction. We have chosen this test case in the belief that it is a stringent test of the method, including all of the essential elements which will be necessary for yet more refined calculations in the future. We have used a modification of the Reid soft core interaction,[14] which was employed in earlier studies of nuclear matter.[4] It is simply the Reid interaction without the $L\cdot S$ interaction terms. We emphasize that the method we have developed can be used to treat still more realistic two- and three-body interactions. However, we believe that the Reid V6 potential is an important first step in treating these systems. The potential may be written as

$$V(r_{ij})=\sum_k v^k(r_{ij})O_{ij}^k \tag{1.1}$$

with the operators O:

$$O_{ij}^k=1,\sigma_i\cdot\sigma_j,\tau_i\cdot\tau_j,\sigma_i\cdot\sigma_j\tau_i\cdot\tau_j,S_{ij},S_{ij}\tau_i\cdot\tau_j \quad \text{for } k=1,6\ . \tag{1.2}$$

The functions v^k depend only upon the distance r_{ij} between particles i and j.

Previous variational calculations in both light nuclei and nuclear matter have indicated that the symmetrized product[5] and independent pair wave functions[6,15] provide accurate descriptions of many nuclear properties. The symmetrized product wave function is given by the expression

$$\Psi=S\left[\prod_{i<j}F_{ij}\right]A\,|\,\Phi\rangle\ , \tag{1.3}$$

where S and A indicate symmetrization and antisymmetrization operators, respectively. The terms F_{ij} are spin-isospin-dependent pair correlation functions of the form

$$F_{ij}=f^c(r_{ij})\left[1+\sum_{k>1}u^k(r_{ij})O_{ij}^k\right]\ . \tag{1.4}$$

The f^c and u^k are functions of the pair separation r_{ij}, and the operators O_{ij}^k are the same as those included in the potential. The correlations are those used in studies of nuclear matter; they are chosen to satisfy the two-body Schrödinger-like equations of Ref. 4. These equations are solved in the spin singlet channels to determine $f_{S=0,T}$ and in the coupled spin triplet channels to determine $f_{S=1,T}$ and $f_{\tau,T}$. The correlation functions are then recombined into the operator form given above. These equations have the form

$$-\frac{\hbar^2}{m}[\phi_{S,T}\nabla^2 f_{S,T}+2\nabla\phi_{S,T}\cdot\nabla f_{S,T}]+[\lambda_{S,T}+v_{S,T}]f_{S,T}\phi_{S,T}=0 \tag{1.5}$$

in the singlet channels and

$$-\frac{\hbar^2}{m}[\phi_{S,T}\nabla^2 f_{S,T}+2\nabla\phi_{S,T}\cdot\nabla f_{S,T}]+[\lambda_{S,T}+v_{S,T}]f_{S,T}\phi_{S,T}+8[\lambda_{t,T}+v_{t,T}]f_{t,T}\phi_{S,T}=0\ , \tag{1.6}$$

$$-\frac{\hbar^2}{m}\left[\phi_{S,T}\nabla^2 f_{t,T}+2\nabla\phi_{S,T}\cdot\nabla f_{t,T}-\frac{6}{r^2}f_{t,T}\phi_{S,T}\right]+[\lambda_{S,T}+v_{S,T}-2(\lambda_{t,T}+v_{t,T})]f_{t,T}\phi_{S,T}+[\lambda_{t,T}+v_{t,T}]f_{S,T}\phi_{S,T}=0 \tag{1.7}$$

in the triplet channels. $\phi_{S,T}$ is given by $[1-(-1)^{S+T}l^2(k_f r)]^{1/2}$, where l is the Slater function and k_f is taken to be a variational parameter. The boundary conditions imposed upon the correlations require that the central correlation f^c heal to 1 and all noncentral correlations u^k be zero beyond a distance d, which is a variational parameter of the wave function.

$A\mid\Phi\rangle$ is a Slater determinant of single particle states, chosen so that the wave function has the correct total angular momentum:

$$\Phi=\prod_{i=1,A}\phi(r_{i,\mathrm{c.m.}})\chi(\sigma_i)\chi(\tau_i)\ . \tag{1.8}$$

These single particle states are functions of the distance of particle i from the center of mass $r_{i,\mathrm{c.m.}}$ and the particle spin σ_i and isospin τ_i. The single particle states $\phi(r)$ for the oxygen nucleus are simply the s- and p-wave bound states of a Woods-Saxon well:

$$V(r)=\frac{V_0}{1+\exp[(r-r_0)/a_0]}\ . \tag{1.9}$$

V_0 is adjusted to give a binding energy E_0 for the p-shell orbitals, and the same well is used to determine the s-wave orbitals. The energy E_0, as well as the radius r_0 and skin thickness a_0 of the well, are also variational parameters.

Variational calculations are performed with the independent pair wave function, which is given by the expression

$$\mid\Psi\rangle=\left[\prod_{i<j}f_{ij}^c(r_{ij})\right]\left[1+\sum_{i<j}\sum_k u^k(r_{ij})O_{ij}^k+\sum_{i<j,l<m}\sum_{k,k'}u^k(r_{ij})u^{k'}(r_{lm})O_{ij}^k O_{lm}^{k'}+\cdots\right]A\mid\Phi\rangle\ . \tag{1.10}$$

This wave function includes correlations over a restricted set of those present in the symmetrized product wave function; the sums exclude products of noncommuting operators. Although this truncated wave function gives slightly higher energies in light nuclei,[6] its simplicity provides a great advantage, so we will use it in the initial studies described here.

II. METHOD

For a nuclear system with realistic interaction and wave function, calculating the expectation value of the Hamiltonian is extraordinarily difficult. Each pair correlation in the wave function is a matrix of $[2^A A!/(Z!N!)]^2$ ($\approx 10^{18}$ for oxygen) elements, and there are $A(A-1)/2$ such correlations. Even though each correlation matrix is sparse, it is not possible to make a full evaluation of the product of correlations at many points in configuration space in order to perform a variational calculation.

Therefore, in order to determine the expectation value of an operator, it is necessary to develop an algorithm which allows the various spin-isospin states of the system to be sampled in the Monte Carlo sense instead of explicitly summed. In this section we first present a general description of the method which we have developed, and then discuss the details of the calculation for nuclear systems.

The major difficulty encountered in sampling over the spin states is the tremendous increase in the statistical error that occurs if this sampling is done in a naive way. In order to reduce the variance, the spin states must be treated in a manner analogous to that commonly used for the spatial coordinates of the system. That is, we try explicitly to select at random from a specific subset of spin-isospin states in a way that, for the exact wave function, gives a zero-variance result for the expectation value of the energy. In order to do this, we observe that the expectation value of the Hamiltonian may be written as

$$\langle H\rangle=\frac{\int dR\sum_{a,b}\Psi_a^\dagger(R)H_{ab}\Psi_b(R)}{\int dR\sum_a\Psi_a^\dagger(R)\Psi_a(R)}\ , \tag{2.1}$$

where R is a $3A$-dimensional vector representing the spatial coordinates of the particles, and a and b represent spin-isospin states. For simplicity, we consider the basis of spin-isospin states to be the set of states for which each particle has a definite third component of spin and isospin. The calculation proceeds by sampling values of R and a, while explicitly summing over all spin-isospin states b for each choice of R and a. The full summation over b, although it is a lengthy computation, greatly reduces the statistical error of the calculation, since for the exact wave function

$$\sum_b H_{ab}\Psi_b = E\Psi_a \tag{2.2}$$

for any values of R and a.

In order to sample R and a efficiently in the combined coordinate-spin-isospin space of the system, we use a generalized version of the standard Metropolis technique of variational Monte Carlo calculations. The result of this random walk is a set of configurations with a probability density proportional to the square of the magnitude of $\Psi_a(R)$.

In this type of walk, instead of simply moving the particles in coordinate space, we must also allow them to change the orientation of the spins and isospins. This may be accomplished, for example, by flipping the third component of the spin of a particle (designated by the operator f_i^σ), or by exchanging two particles's spin and isospin ($P_{ij}^\sigma P_{ij}^\tau$). In the latter case, a proposed Metropolis step may consist of choosing a new value R' for a particle i in the standard manner and new values of a' by

$$a' = P_{ij}^\sigma P_{ij}^\tau(a) \ , \tag{2.3}$$

where j is chosen randomly among the particles. The proposed move is accepted or rejected according to the ratio of the squares of the wave functions evaluated at (R,a) and (R',a'), as in standard variational Monte Carlo. As long as detailed balance is preserved and the entire coordinate-spin-isospin space of the problem is spanned, any type or combination of types of Metropolis steps may be chosen.

In these studies, we have combined the two types of steps. Half of the steps are taken using the spin-flip operator to sample the spin-isospin space, and the other half using a spin-isospin exchange operator. In principle, the walk could be undertaken using only a spin flip to traverse the spin space. However, we find that these steps have a relatively low acceptance rate of around 10 percent, so the combination of different steps is preferable.

As the walk progresses the expectation value of any operator O may be evaluated from the expression

$$\langle O \rangle = \frac{1}{N}\sum_i \frac{\Psi_{a_i}^\dagger(R_i)\sum_b O_{a_i b}\Psi_b(R_i)}{\Psi_{a_i}^\dagger(R_i)\Psi_{a_i}(R_i)} \ , \tag{2.4}$$

where the sum from i is a sum over the set of N configurations with coordinates R_i and a_i. Different formulations for $\langle O \rangle$ are possible.

This prescription would be adequate to handle many problems, but is insufficient in itself to treat nuclear systems with realistic interactions. In these systems, it is extremely difficult to calculate even one spin-isospin component of the wave function exactly, due to the extremely large number of spin dependent correlations in the independent pair wave function.

We proceed in the same spirit invoked above, namely to compute what can be done explicitly and which contributes the most, and sample the rest. Here that will mean computing explicitly terms through order u^2 in the expansion of Ψ [Eq. (1.10)] and random sampling of representative terms with higher powers of u. The terms of order u^2 and lower represent a large fraction of the normalization of the wave function, so it is important to include them fully and exactly. The symmetries of Φ and the fact that many pairs are separated by a distance greater than the correlation length make this evaluation feasible. The higher order terms do make significant contributions to the energy, however, so realistic calculations must take them into account through a sampling procedure.

In order to sample these higher order terms in the independent pair wave function, an efficient scheme is required. We first choose a random set of $A/2$ pairings such that each particle is paired with exactly one other particle. The contribution of all terms of order u^3 and higher to the matrix element

$$M = \left\langle a \left| \prod_{\text{pairs}} \left[1 + \sum_k u^k(r_{ij}) O_{ij}^k \right] \right| \Phi \right\rangle \tag{2.5}$$

is then determined through a sampling procedure. The matrix element M may be written as the sum of matrix elements M^N, where M^N is the contribution from all terms in the product with exactly N noncentral correlations. We wish to evaluate M^N for $N=3$ to $A/2$.

In general, many of the $A/2$ pairs will be separated by a distance greater than the healing distance of the correlation, and hence will be uncorrelated. Thus, only those spin-isospin components of Φ in which these particles's spins and isospins are unchanged will contribute to M. Nevertheless, there is a very large number of components of Φ that satisfy this condition. A subset of the components is chosen and all M^N are evaluated, for $N=3$ to $A/2$. In order to correct for the fact that we have not included all components of Φ, the matrix elements M^N are multiplied by the ratio of the total number of components of Φ which contribute to M to the number contained in the subset.

This entire procedure is repeated many times with different choices for the pairings. The results are then averaged, resulting in a value for each M^N. In order to calculate the contribution to the wave function, each M^N is multiplied by the ratio of the total number of terms in the independent pair wave function with exactly N noncentral correlations to the number of those terms which have been evaluated. As an example, assume we wished to determine the contribution of the linear terms in u to the wave function with this method. Each pairing of the particles produces $A/2$ contributions to M^1. There are, however, $A(A-1)/2$ terms with exactly one noncentral correlation in the independent pair wave function, and therefore multiplying the average value of M^1 by $A-1$ gives the correct contribution of the u^1 terms.

The process of pairing the $A/2$ particles is chosen because this ratio is reasonable for all values of N, so that it is feasible to calculate the contribution of many terms in this manner. The average value of the sum of these contributions is equal to the contribution of all terms of order u^3 and higher to the wave function.

Since we want to take the walk with a probability distribution proportional to $\Psi^\dagger\Psi$, this sampling procedure is carried out independently for Ψ and $\Psi^\dagger$. With the inclusion of these sampled terms, the product $\Psi^\dagger\Psi$ is no longer positive definite, so the weight for the random walk is taken as the product of the magnitude of Ψ by the magnitude of $\Psi^\dagger$:

$$W_a(R) = |\Psi_a^\dagger(R)|\ |\Psi_a(R)|\ . \tag{2.6}$$

The expectation value of the Hamiltonian may then be written as

$$\langle O \rangle = \frac{\displaystyle\sum_i \frac{\Psi_{a_i}^\dagger(R_i)\sum_b O_{a_i b}\Psi_b(R_i)}{W_{a_i}(R_i)}}{\displaystyle\sum_i \frac{\Psi_{a_i}^\dagger(R_i)\Psi_{a_i}(R_i)}{W_{a_i}(R_i)}}\ . \tag{2.7}$$

The matrix elements of both the kinetic and potential energy are determined as in Eq. (2.7). The derivatives necessary to calculate the kinetic energy are calculated numerically.

In order to evaluate the potential energy, a sum over all pairs of particles is required. This sum involves a large number of spin-isospin components b. In order to increase the efficiency of the calculation, only a subset of pairs is evaluated for every configuration. Pairs to be included are chosen with probability $p(r_{ij})$,

$$\begin{aligned} p(r_{ij}) &= 1 \quad \text{for } r_{ij} < 1.5 \text{ fm} \\ &= \exp[-0.7(r_{ij}-1.5)] \quad \text{for } r_{ij} > 1.5 \text{ fm}\ , \end{aligned} \tag{2.8}$$

and given an additional weight factor $1/p$. In this way, all nearby pairs of particles are evaluated explicitly, while well-separated pairs are evaluated rarely.

A typical variational run involves several thousand energy evaluations, with the computer time divided roughly equally between calculation of the kinetic and potential energy. Also, the time spent calculating lower order terms (through u^2) is comparable to the time spent sampling the higher order terms.

III. RESULTS

We have calculated several properties of the ground state of ^{16}O, including the total energy, charge radius, and form factor. Our results are summarized in Tables I—III and Figs. 1—3.

The set of variational parameters which produces the minimum energy is given in Table I. The calculations are very time consuming so the parameters have not been fully optimized. The correlation length and the depth and radius of the Woods-Saxon well are the most sensitive parameters; changes in these parameters produce the largest changes in the total energy.

Prior to performing calculations with the complete independent pair wave function, we calculated various properties of the system with wave functions containing only the linear or linear-plus-quadratic terms in the noncentral correlations. A comparison of these results is presented in Table II. The total energies obtained with these simplistic wave functions are not accurate. The minimum energy for the linear and linear-plus-quadratic wave functions are only about -1 MeV and -4 MeV per particle, respectively. However, a large fraction of the total kinetic and potential energies is present in these wave functions. It is for this reason that these terms are calculated explicitly, rather than sampled. These preliminary calculations also proved useful in giving a guide for determining the variational parameters.

As is apparent from Table II, the error in the total energy increases rapidly when the higher order terms are included. This fact points toward a need for more efficient sampling of these terms. An increase in efficiency by

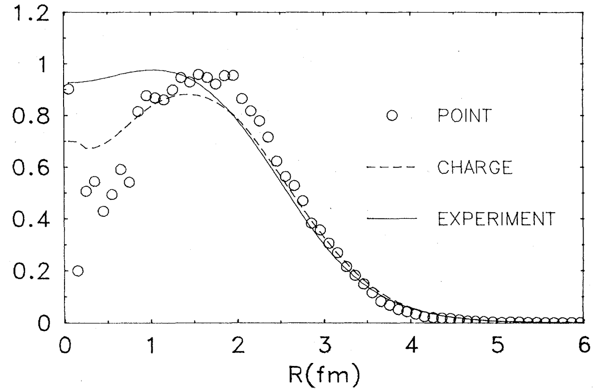

FIG. 1. Charge distribution of ^{16}O, calculated and experimental (Ref. 16). The circles indicate the point proton distribution. These points are folded with the proton charge distribution to obtain the solid curve.

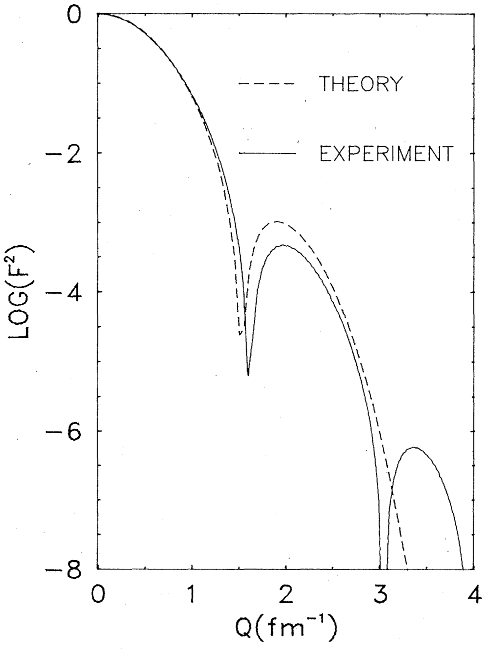

FIG. 2. Charge form factor of ^{16}O calculated in the impulse approximation and experimental results (Ref. 16).

TABLE I. Variational parameters.

Parameter	Value	
d	2.5	fm
E_0	13.0	MeV
r_0	3.5	fm
a_0	0.25	fm
k_f	1.1	fm^{-1}

roughly a factor of 10 (which would decrease the error by a factor of 3) will be necessary to yield detailed information about the energy of the system. Such a factor does not seem out of reach as computational facilities improve and further refinements are made in the algorithm.

Results of several calculations with the independent pair wave function are listed in Table III. A correlation length of roughly 2.5 fm appears to be optimal. This is somewhat larger than the minimum value obtained for nuclear matter at equilibrium density, approximately 2.1 fm for a very similar parametrization. As expected, the magnitude of both the kinetic and potential energies increases as the correlation length is increased. It is very difficult to make fine distinctions in various parameters, however, as the statistical errors are relatively large.

The minimum energy which we obtained with the Reid V6 interaction is -7.0 ± 1.3 MeV per nucleon. The Coulomb energy for this system is approximately 0.8 MeV per nucleon, so the total energy is -6.2 as compared with an experimental value of -8. It is not apparent from these initial studies what portion of the difference is due to our choice of variational wave function and what part is due to the simplified form of the interaction. Future studies should determine the importance of using more realistic two- and three-body interactions.

The rms charge radius of our wave function is 2.72 ± 0.05 fm, in good agreement with the experimental value of 2.70 ± 0.02. We have also calculated the charge distribution and the charge form factor. The charge distribution is given in Fig. 1, and the charge form factor in Fig. 2. Each is compared with the experimental results of Sick *et al.*[16]

In Fig. 1, the circles represent the point proton distribution, and the dashed line gives the charge distribution, which is obtained by folding the point particle distribution with the nucleon charge density. The curves agree well except at small values of r (<1.5 fm), where the calculated charge density is considerably smaller than the experimental results would indicate. Equivalently, the charge form factor agrees very well with the experimental results at small q, but disagrees at larger values of the momentum transfer.

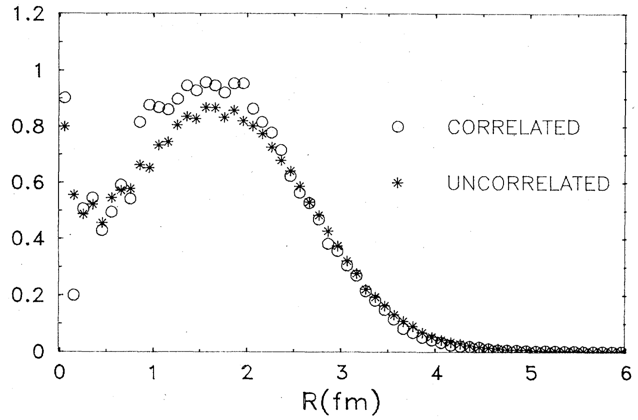

FIG. 3. A comparison of the point proton distribution of the full independent pair wave function and the uncorrelated Φ.

The discrepancy between theoretical and experimental charge distributions at small radii arises from the choice of variational wave function and possibly from the neglect of exchange current contributions to the charge form factor. Since all of the single particle states in Φ are functions of the distance to the center of mass, the 12 nucleons in the p shell are excluded from this region.

The central depression in the point distribution is apparent in the experimental results, as there is a central depression in the charge density. This depression indicates a greater reduction in the equivalent point nucleon distribution at the center of mass, but the experiments would predict a much smaller effect. Also, the inclusion of meson exchange currents will significantly alter the calculated form factor, and consequently the charge distribution. The exchange current contributions are quite large, especially in the region of the second diffraction minimum.[17]

Finally, a comparison of the charge distribution with and without correlations is presented in Fig. 3. There is little difference between the two distributions, except for a small decrease in the rms radius caused by the correlations. Previous shell model calculations indicated that it might be necessary to include pair correlations in the wave function in order to reproduce the second diffraction minimum in the charge form factor.[18] Simple harmonic oscillator shell model wave functions without center of mass corrections will not produce a second minimum, but on the basis of our work it seems unlikely that this feature

TABLE II. Results for linear, linear-plus-quadratic, and full independent pair (IP) wave functions. Variational parameters other than d are given in Table I. These values are near the variational minimum for each type of wave function.

Type	d	E	T	V	$\langle r_p^2\rangle^{1/2}$ [a]
Linear	2.25	-12 ± 6	343 ± 9	-355 ± 15	2.68
Quadratic	2.50	-58 ± 9	417 ± 10	-474 ± 15	2.62
IP	2.50	-112 ± 18	414 ± 11	-525 ± 22	2.60

[a] $\langle r_p^2\rangle^{1/2}$ is the root mean square radius of the point proton distribution.

TABLE III. Results for full independent pair (IP) wave functions.

Type	d	E	T	V	$\langle r_p^2 \rangle^{1/2\,a}$
IP	2.30	-77 ± 13	382 ± 14	-459 ± 18	2.69
IP	2.50	-112 ± 18	414 ± 11	-525 ± 22	2.60
IP	2.60	-75 ± 18	445 ± 29	-521 ± 25	2.59

[a] $\langle r_p^2 \rangle^{1/2}$ is the root mean square radius of the point proton distribution.

can be explicitly tied to the presence of correlations. Correlations may, however, play a significant role in determining fine details of nuclear charge distributions, especially in areas such as the difference between nearby nuclei. Future investigations in this area may prove very useful.

IV. CONCLUSIONS

We believe that this variational Monte Carlo method will prove to be very valuable for microscopic calculations of large nuclei with realistic interactions. The calculations presented in this paper are an important first step in this direction. In order to realize this goal more fully, several aspects of the method should be improved.

The large computational times can be reduced by improving the efficiency of the sampling algorithm for the higher order terms, which is the limiting factor at present. An improvement of roughly an order of magnitude seems feasible in this area. Also, it would be very desirable to extend the method to use the full symmetrized product wave function.

Alternatively, one could investigate different choices for the variational wave function. We have chosen the extreme single-particle model for our uncorrelated state Φ in this work. While this is conceptually attractive, it is computationally difficult, since the wave function then requires rather long range spin dependent pair correlations in order to minimize the energy. The calculation of these correlations dominates the calculation of the energy. Therefore, it may be profitable to include a less restricted shell model state as the uncorrelated wave function.

This work has shown that it is feasible to perform realistic variational Monte Carlo calculations on *p*-shell nuclei. Variational calculations may prove to be of significant value in improving our understanding of many aspects of nuclear structure.

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