RECEIVED
OCT 24 1997
OSTI

CONF-970731--

1

RECEIVED

NOV 10 1997

OSTI

Quantum Monte Carlo calculations for light nuclei

R. B. Wiringa^{a*}

^aPhysics Division, Argonne National Laboratory,
Argonne, IL 60439, USA

Quantum Monte Carlo calculations of ground and low-lying excited states for nuclei with $A \leq 8$ have been made using a realistic Hamiltonian that fits NN scattering data. Results for more than two dozen different (J^π, T) p -shell states, not counting isobaric analogs, have been obtained. The known excitation spectra of all the nuclei are reproduced reasonably well. Density and momentum distributions and various electromagnetic moments and form factors have also been computed. These are the first microscopic calculations that directly produce nuclear shell structure from realistic NN interactions.

1. INTRODUCTION

Quantum Monte Carlo calculations [1,2] of ground and low-lying excited states for nuclei with $A \leq 8$ have been made using a realistic Hamiltonian containing the Argonne v_{18} two-nucleon and Urbana IX three-nucleon potentials [3]. The first step in these calculations is the construction of a variational wave function, $\Psi_V(J^\pi, T)$, using products of two- and three-body correlation operators acting on a fully antisymmetrized set of one-body p -shell basis states coupled to the specified quantum numbers. Metropolis Monte Carlo integration is used to evaluate $\langle \Psi_V | H | \Psi_V \rangle$ and diagonalize in the one-body p -shell basis, giving an upper bound to the lowest state with these quantum numbers. The Ψ_V is then used as input to the Green's function Monte Carlo algorithm, which projects out excited state contamination in the trial wave function by the Euclidean propagation $\Psi(\tau) = \exp[-(H - E_0)\tau]\Psi_V$. In the limit $\tau \rightarrow \infty$, this yields the exact $\Psi_0(J^\pi, T)$, but in practice the propagation is limited to $\tau \leq 0.06 \text{ MeV}^{-1}$. Nevertheless, the transient energy, $E(\tau) = \langle \Psi_V | H | \Psi(\tau) \rangle$ gives a significantly improved upper bound compared to the variational result, which we estimate to be within $\sim 1\%$ of the exact binding energy for this Hamiltonian.

We obtain ground states of both ${}^6\text{Li}$ and ${}^7\text{Li}$ that are stable against breakup into subclusters, but somewhat underbound compared to experiment. Results for many additional states in ${}^6\text{He}$, ${}^7\text{He}$, ${}^8\text{He}$, ${}^8\text{Li}$, and ${}^8\text{Be}$ have also been obtained. The known excitation spectra of all these nuclei are reproduced reasonably well and a number of excited states in ${}^6\text{He}$ and ${}^7\text{He}$ are predicted. We have also computed energy differences between isobaric analogs to study the charge-independence-breaking of the strong and electromagnetic forces. A variety of density and momentum distributions are also computed, along with electro-

*This work supported by the U. S. Department of Energy, Nuclear Physics Division, under contract No. W-31-109-ENG-38.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

**Portions of this document may be illegible
in electronic image products. Images are
produced from the best available original
document.**

magnetic moments, and form factors. These are the first microscopic calculations that directly produce nuclear shell structure from realistic interactions that fit NN scattering data.

2. HAMILTONIAN

Our Hamiltonian includes a nonrelativistic one-body kinetic energy, the Argonne v_{18} two-nucleon potential [3] and the Urbana IX three-nucleon potential [1],

$$H = \sum_i K_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} . \quad (1)$$

The kinetic energy operator has charge-independent (CI) and charge-symmetry-breaking (CSB) components, the latter due to the difference in proton and neutron masses,

$$K_i = K_i^{CI} + K_i^{CSB} \equiv -\frac{\hbar^2}{4} \left(\frac{1}{m_p} + \frac{1}{m_n} \right) \nabla_i^2 - \frac{\hbar^2}{4} \left(\frac{1}{m_p} - \frac{1}{m_n} \right) \tau_{zi} \nabla_i^2 . \quad (2)$$

The Argonne v_{18} potential can be written as a sum of electromagnetic and one-pion-exchange terms and a shorter-range phenomenological part,

$$v_{ij} = v_{ij}^\gamma + v_{ij}^\pi + v_{ij}^R . \quad (3)$$

The electromagnetic terms include one- and two-photon-exchange Coulomb interaction, vacuum polarization, Darwin-Foldy, and magnetic moment terms, with appropriate proton and neutron form factors:

$$v^\gamma(pp) = V_{C1}(pp) + V_{C2} + V_{VP} + V_{DF} + V_{MM}(pp) , \quad (4)$$

$$v^\gamma(np) = V_{C1}(np) + V_{MM}(np) , \quad (5)$$

$$v^\gamma(nn) = V_{MM}(nn) . \quad (6)$$

The V_{MM} contain spin-spin, tensor, and spin-orbit components. Detailed expressions for these terms, including the form factors, are given in Ref. [3].

The one-pion-exchange part of the potential includes the charge-dependent (CD) terms due to the difference in neutral and charged pion masses. It can be written as

$$v_{ij}^\pi = f^2 \left(\frac{m}{m_s} \right)^2 \frac{1}{3} m c^2 \left[X_{ij} \tau_i \cdot \tau_j + \tilde{X}_{ij} T_{ij} \right] , \quad (7)$$

where $T_{ij} = 3\tau_{zi}\tau_{zj} - \tau_i \cdot \tau_j$ is the isotensor operator and

$$X_{ij} = \frac{1}{3} \left(X_{ij}^0 + 2X_{ij}^\pm \right) , \quad (8)$$

$$\tilde{X}_{ij} = \frac{1}{3} \left(X_{ij}^0 - X_{ij}^\pm \right) , \quad (9)$$

$$X_{ij}^m = [Y(mr_{ij})\sigma_i \cdot \sigma_j + T(mr_{ij})S_{ij}] . \quad (10)$$

Here $Y(x)$ and $T(x)$ are the normal Yukawa and tensor functions with a cutoff specified in Ref. [3], and $X^{\pm,0}$ are calculated with $m = m_{\pi^\pm}$ and m_{π^0} .

The one-pion-exchange and the remaining phenomenological part of the potential can be written as a sum of eighteen operators,

$$v_{ij}^\pi + v_{ij}^R = \sum_{p=1,18} v_p(r_{ij}) O_{ij}^p . \quad (11)$$

The first fourteen are charge-independent,

$$O_{ij}^{p=1,14} = [1, (\sigma_i \cdot \sigma_j), S_{ij}, (\mathbf{L} \cdot \mathbf{S}), \mathbf{L}^2, \mathbf{L}^2(\sigma_i \cdot \sigma_j), (\mathbf{L} \cdot \mathbf{S})^2] \otimes [1, (\tau_i \cdot \tau_j)] , \quad (12)$$

while the last four,

$$O_{ij}^{p=15,18} = [1, (\sigma_i \cdot \sigma_j), S_{ij}] \otimes T_{ij}, (\tau_{zi} + \tau_{zj}) , \quad (13)$$

break charge independence. We will refer to the potential from the $p = 15 - 17$ terms as v^{CD} and from the $p = 18$ term as v^{CSB} . There could in principle be more charge-independence-breaking (CIB) terms such as $\mathbf{L} \cdot \mathbf{S} T_{ij}$ or $S_{ij}(\tau_{zi} + \tau_{zj})$ but the scattering data are not sufficiently precise to identify them at present.

The potential was fit directly to the Nijmegen NN scattering data base [4,5] containing 1787 pp and 2514 np data in the range 0 – 350 MeV, with a χ^2 per datum of 1.09. It was also fit to the nn scattering length measured in $d(\pi^-, \gamma)nn$ experiments and the deuteron binding energy.

The Urbana series of three-nucleon potentials is written as a sum of two-pion-exchange and shorter-range phenomenological terms,

$$V_{ijk} = V_{ijk}^{2\pi} + V_{ijk}^R . \quad (14)$$

The two-pion-exchange term can be expressed simply as

$$V_{ijk}^{2\pi} = \sum_{cyclic} A_{2\pi} \{X_{ij}^\pi, X_{jk}^\pi\} \{\tau_i \cdot \tau_j, \tau_j \cdot \tau_k\} + C_{2\pi} [X_{ij}^\pi, X_{jk}^\pi] [\tau_i \cdot \tau_j, \tau_j \cdot \tau_k] , \quad (15)$$

where X_{ij}^π is constructed with an average pion mass, $m_\pi = \frac{1}{3}m_{\pi^0} + \frac{2}{3}m_{\pi^\pm}$. The anticommutator and commutator terms are denoted by V_{ijk}^A and V_{ijk}^C , respectively, and for the Urbana models $C_{2\pi} = \frac{1}{4}A_{2\pi}$, as in the original Fujita-Miyazawa model [6]. The shorter-range phenomenological term is given by

$$V_{ijk}^R = \sum_{cyclic} U_0 T^2(m_\pi r_{ij}) T^2(m_\pi r_{jk}) . \quad (16)$$

The parameters have been determined by fitting the density of nuclear matter and the binding energy of ^3H in conjunction with the Argonne v_{18} interaction. In principle, the V_{ijk}^R can have other terms [7], however we need additional data to obtain their strengths; presumably a part of it is due to relativistic effects [8,9].

Direct GFMC calculations with the full interaction (in particular spin-dependent terms which involve the square of the momentum operator) have very large statistical errors. Also the CIB terms in H are fairly weak and therefore can be treated conveniently as a first order perturbation. Further, using a wave function of good isospin significantly reduces the cost of the calculations. Hence we construct the GFMC propagator with a simpler isoscalar Hamiltonian,

$$H' = \sum_i K_i^{CI} + \sum_{i<j} v'_{ij} + \sum_{i<j<k} V'_{ijk} , \quad (17)$$

where v'_{ij} is defined as

$$v'_{ij} = \sum_{p=1,8} v'_p(r_{ij}) O_{ij}^p + v'_C(r_{ij}) . \quad (18)$$

The interaction v'_{ij} has only eight operator terms, with operators $[1, (\sigma_i \cdot \sigma_j), S_{ij}, (\mathbf{L} \cdot \mathbf{S})] \otimes [1, (\tau_i \cdot \tau_j)]$, chosen such that it equals the isoscalar part of the full interaction in all S and P waves as well as in the 3D_1 wave and its coupling to the 3S_1 . The isoscalar part of $V_{C1}(pp)$ is also included in H' .

The v'_{ij} is a little more attractive than v_{ij} — about 2 MeV extra binding in ${}^4\text{He}$. We compensate for this tendency towards overbinding by using a V'_{ijk} in which the repulsive U_0 term of Eq.(16) has been increased by $\sim 30\%$. This ensures $\langle H' \rangle \approx \langle H \rangle$ so that the GFMC propagation does not produce excessively large densities due to overbinding. The contribution of $\langle H - H' \rangle$ is calculated perturbatively.

3. VARIATIONAL MONTE CARLO

The variational method can be used to obtain approximate solutions to the many-body Schrödinger equation, $H\Psi = E\Psi$, for a wide range of nuclear systems, including few-body nuclei, light closed shell nuclei, nuclear matter, and neutron stars [10]. A suitably parameterized wave function, Ψ_V , is used to calculate an upper bound to the exact ground-state energy,

$$E_V = \frac{\langle \Psi_V | H | \Psi_V \rangle}{\langle \Psi_V | \Psi_V \rangle} \geq E_0 . \quad (19)$$

The parameters in Ψ_V are varied to minimize E_V , and the lowest value is taken as the approximate ground-state energy.

Upper bounds to excited states are also obtainable, either from standard VMC calculations if they have different quantum numbers from the ground state, or from small-basis diagonalizations if they have the same quantum numbers. The corresponding Ψ_V can then be used to calculate other properties, such as particle density or electromagnetic moments, or it can be used as the starting point for a Green's function Monte Carlo calculation. In this section we first describe our *ansatz* for Ψ_V for the light p -shell nuclei and then briefly review how the expectation value, Eq.(19), is evaluated and the parameters of Ψ_V are fixed.

Our best variational wave function for the nuclei studied here has the form [11]

$$|\Psi_V\rangle = \left[1 + \sum_{i<j<k} (U_{ijk} + U_{ijk}^{TNI}) + \sum_{i<j} U_{ij}^{LS} \right] |\Psi_P\rangle , \quad (20)$$

where the pair wave function, Ψ_P , is given by

$$|\Psi_P\rangle = \left[\mathcal{S} \prod_{i<j} (1 + U_{ij}) \right] |\Psi_J\rangle . \quad (21)$$

The U_{ij} , U_{ij}^{LS} , U_{ijk} , and U_{ijk}^{TNI} are noncommuting two- and three-nucleon correlation operators, and the $\mathcal{S}$ is a symmetrization operator. The form of the totally antisymmetric Jastrow wave function, Ψ_J , depends on the nuclear state under investigation. For the s -shell nuclei we use the simple form

$$|\Psi_J\rangle = \left[\prod_{i<j<k} f_{ijk}^c \right] \left[\prod_{i<j} f_c(r_{ij}) \right] |\Phi_A(JMTT_3)\rangle. \quad (22)$$

Here $f_c(r_{ij})$ and f_{ijk}^c are central two- and three-body correlation functions and

$$|\Phi_3(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2})\rangle = \mathcal{A}|p \uparrow p \downarrow n \uparrow\rangle, \quad (23)$$

$$|\Phi_4(0000)\rangle = \mathcal{A}|p \uparrow p \downarrow n \uparrow n \downarrow\rangle. \quad (24)$$

The two-body correlation operator U_{ij} is a sum of spin, isospin, and tensor terms:

$$U_{ij} = \sum_{p=2,6} \left[\prod_{k \neq i,j} f_{ijk}^p(\mathbf{r}_{ik}, \mathbf{r}_{jk}) \right] u_p(r_{ij}) O_{ij}^p, \quad (25)$$

while the two-body spin-orbit correlation operator is given by

$$U_{ij}^{LS} = \sum_{p=7,8} u_p(r_{ij}) O_{ij}^p. \quad (26)$$

The U_{ij} and U_{ij}^{LS} correlations are induced by the two-nucleon interaction. The equations used to generate the functions $f_c(r_{ij})$ and $u_p(r_{ij})$ are given in Ref. [12]; they contain a number of variational parameters to be determined by minimizing the energy.

The f_{ijk}^c , f_{ijk}^p , and U_{ijk} are three-nucleon correlations induced by v_{ij} . The first two have an operator-independent form, while the U_{ijk} involve additional spin-isospin operators and are somewhat more complicated; they are discussed in Ref. [11]. The U_{ijk}^{TNI} are three-body correlations induced by the three-nucleon interaction, which we take in the form suggested by perturbation theory:

$$U_{ijk}^{TNI} = \sum_x \epsilon_x V_{ijk}^x(\tilde{r}_{ij}, \tilde{r}_{jk}, \tilde{r}_{ki}), \quad (27)$$

with $\tilde{r} = yr$, y a scaling parameter, and ϵ_x a strength parameter. Here $x = A, C$, and R refers to the different parts of the NNN potential. A somewhat simpler wave function to evaluate, is given by:

$$|\Psi_T\rangle = \left[1 + \sum_{i<j<k} \tilde{U}_{ijk}^{TNI} \right] |\Psi_P\rangle, \quad (28)$$

where $\tilde{U}_{ijk}^{TNI}$ is a truncated TNI correlation from which the commutator term, $\epsilon_C V_{ijk}^C$, has been omitted. The Ψ_T gives about 1–2 MeV less binding than the full Ψ_V , but costs less than half as much computationally, and it actually makes a more efficient starting point for the GFMC calculation.

The Jastrow wave function for $A = 6$ nuclei is more complicated, as two nucleons must be placed in the p -shell. We use LS coupling to obtain the desired JM value of a given state, as suggested in shell-model studies of p -shell nuclei [13]. Different possible LS combinations lead to multiple components in the Jastrow wave function. We also allow for the possibility that the central correlations $f_c(r_{ij})$ and f_{ijk}^c could depend upon

the shells (*s* or *p*) occupied by the particles and on the *LS* coupling. The Jastrow wave function is taken as

$$|\Psi_J\rangle = \mathcal{A} \left\{ \left[\prod_{i < j < k \leq 4} f_{ijk}^{sss} \prod_{l < m \leq 4} f_{lm5}^{ssp} f_{lm6}^{ssp} \prod_{n \leq 4} f_{n56}^{spp} \right] \left[\prod_{i < j \leq 4} f_{ss}(r_{ij}) \prod_{k \leq 4} f_{sp}(r_{k5}) f_{sp}(r_{k6}) \sum_{LS} \left(\beta_{LS} f_{pp}^{LS}(r_{56}) |\Phi_6(LSJMTT_3)_{1234:56}\rangle \right) \right] \right\} \quad (29)$$

The operator $\mathcal{A}$ indicates an antisymmetric sum over all possible partitions of the six particles into 4 *s*-shell and 2 *p*-shell ones. For the two-body correlations we use $f_{ss}(r) = f_c(r)$ from the ${}^4\text{He}$ wave function, while the $f_{sp}(r)$ and $f_{pp}(r)$ have a similar shape with a possible long-range tail added. For the three-body correlations, our best present trial function has $f_{ijk}^{sss} = f_{ijk}^c$ as in ${}^4\text{He}$ and $f_{ijk}^{ssp} = f_{ijk}^{spp} = 1$.

The *LS* components of the single-particle wave function are given by:

$$\begin{aligned} |\Phi_6(LSJMTT_3)_{1234:56}\rangle &= |\Phi_4(0000)_{1234}\phi_p^{LS}(R_{\alpha 5})\phi_p^{LS}(R_{\alpha 6}) \\ &\left\{ [Y_{1m_l}(\Omega_{\alpha 5})Y_{1m'_l}(\Omega_{\alpha 6})]_{LM_L} \times [\chi_5(\tfrac{1}{2}m_s)\chi_6(\tfrac{1}{2}m'_s)]_{SM_S} \right\}_{JM} \\ &\times [\nu_5(\tfrac{1}{2}t_3)\nu_6(\tfrac{1}{2}t'_3)]_{TT_3} \rangle. \end{aligned} \quad (30)$$

The $\phi_p^{LS}(R_{\alpha k})$ are *p*-wave solutions of a particle of reduced mass $\frac{4}{5}m_N$ in an effective α -*N* potential. They are functions of the distance between the center of mass of the α core (which contains particles 1-4 in this partition) and nucleon *k*, and again may be different for different *LS* components. We use a Woods-Saxon potential well:

$$V_{\alpha N}(r) = V_p^{LS} [1 + \exp(\frac{r - R_p}{a_p})]^{-1}, \quad (31)$$

where V_p^{LS} , R_p , and a_p are variational parameters.

For $A = 7, 8$ nuclei, the generalization of $|\Psi_J\rangle$ is straightforward, except that with three or more *p*-shell particles there are multiple ways of coupling to obtain the orbital angular momentum, *L*, and spin, *S*, and thus the total (J^π, T) of the system. The spatial permutation symmetry, denoted by the Young pattern $[n]$, is used to enumerate the different possible terms, as discussed in Appendix 1C of Ref. [14]. The different possible contributions to $A = 6 - 8$ nuclei are given in Table 1. For $A = 6 - 7$ nuclei and for ${}^8\text{He}$, we have used a complete *p*-shell basis, but so far only the states with the highest spatial symmetry have been used in ${}^8\text{Li}$ and ${}^8\text{Be}$; those not used are marked by an ‘*’ in the table.

After other parameters in the trial function have been optimized, we make a series of calculations in which the $\beta_{LS[n]}$ of Eq.(29) may be different in the left- and right-hand-side wave functions to obtain the diagonal and off-diagonal matrix elements of the Hamiltonian and the corresponding normalizations and overlaps. We diagonalize the resulting $N \times N$ matrices to find the $\beta_{LS[n]}$ eigenvectors, using generalized eigenvalue routines because the correlated Ψ_V are not orthogonal. This allows us to project out not only the ground states, but excited states of the same (J^π, T) quantum numbers. For example, the ground states of ${}^6\text{Li}$, ${}^7\text{Li}$, and ${}^8\text{Li}$ are obtained from 3×3 , 5×5 , and 4×4 diagonalizations, respectively.

Table 1

Permutation symmetry terms for LS -coupling in $A = 6 - 8$ nuclei

A	$[n]$	L	(T, S)
6	[2]	0, 2	(1, 0)(0, 1)
	[11]	1	(1, 1)(0, 0)
7	[3]	1, 3	$(\frac{1}{2}, \frac{1}{2})$
	[21]	1, 2	$(\frac{3}{2}, \frac{1}{2})(\frac{1}{2}, \frac{3}{2})(\frac{1}{2}, \frac{1}{2})$
	[111]	0	$(\frac{3}{2}, \frac{3}{2})(\frac{1}{2}, \frac{1}{2})$
8	[4]	0, 2, 4	(0, 0)
	[31]	1, 2, 3	(1, 1)(1, 0)(0, 1)*
	[22]	0, 2	(2, 0)(1, 1)*(0, 2)*(0, 0)*
	[211]	1	(2, 1)(1, 2)*(1, 1)*(1, 0)*(0, 1)*

The energy expectation value of Eq.(19) is evaluated using Monte Carlo integration. A detailed technical description of the methods used here can be found in Refs. [12,15,16]. Monte Carlo sampling is done both in configuration space and in the order of operators in the symmetrized product of Eq.(21) by following a Metropolis random walk. The expectation value for an operator O is computed with the expression

$$\langle O \rangle = \frac{\sum_{p,q} \int d\mathbf{R} [\Psi_p^\dagger(\mathbf{R}) O \Psi_q(\mathbf{R}) / W_{pq}(\mathbf{R})] W_{pq}(\mathbf{R})}{\sum_{p,q} \int d\mathbf{R} [\Psi_p^\dagger(\mathbf{R}) \Psi_q(\mathbf{R}) / W_{pq}(\mathbf{R})] W_{pq}(\mathbf{R})}, \quad (32)$$

where a probability distribution, $W_{pq}(\mathbf{R})$, has been introduced. The subscripts p and q specify the order of operators in the left and right hand side wave functions, while the integration runs over the particle coordinates $\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$. The probability distribution is constructed from the Ψ_P of Eq.(21):

$$W_{pq}(\mathbf{R}) = |\text{Re}(\langle \Psi_{P,p}^\dagger(\mathbf{R}) \Psi_{P,q}(\mathbf{R}) \rangle)|. \quad (33)$$

This is much less expensive to compute than using the full wave function of Eq.(20) with its spin-orbit and operator-dependent three-body correlations, but it typically has a norm within 1-2% of the full wave function.

Expectation values have a statistical error which can be estimated by the standard deviation σ :

$$\sigma = \left[\frac{\langle O^2 \rangle - \langle O \rangle^2}{N - 1} \right]^{1/2}, \quad (34)$$

where N is the number of statistically independent samples. Block averaging schemes can be used to estimate the autocorrelation times and determine the statistical error.

The wave function Ψ can be represented by an array of $2^A \times \binom{A}{2}$ complex numbers,

$$\Psi(\mathbf{R}) = \sum_{\alpha} \psi_{\alpha}(\mathbf{R}) |\alpha\rangle, \quad (35)$$

where the $\psi_{\alpha}(\mathbf{R})$ are the coefficients of each state $|\alpha\rangle$ with specific third components of spin and isospin. This gives arrays with 96, 1280, 4480, and 14336 elements for ${}^4\text{He}$, ${}^6\text{Li}$,

${}^7\text{Li}$, and ${}^8\text{B}$, respectively. The spin, isospin, and tensor operators $O_{ij}^{p=2,6}$ contained in the two-body correlation operator U_{ij} , and in the Hamiltonian are sparse matrices in this basis. For forces that are largely charge-independent, as is the case here, we can replace this charge-conserving basis with an isospin-conserving basis that has $N(A, T) = 2^A \times I(A, T)$ components, where

$$I(A, T) = \frac{2T + 1}{\frac{1}{2}A + T + 1} \binom{A}{\frac{1}{2}A + T}. \quad (36)$$

This reduces the number of array elements to 32, 320, 1792, and 7168 for the cases given above—a significant savings. In practice, isospin operators are more expensive to evaluate in this basis, but the overall savings in computation is still large.

Expectation values of the kinetic energy and spin-orbit potential require the computation of first derivatives and diagonal second derivatives of the wave function. These are obtained by evaluating the wave function at $6A$ slightly shifted positions of the coordinates $\mathbf{R}$ and taking finite differences, as discussed in Ref. [12]. Potential terms quadratic in $\mathbf{L}$ require mixed second derivatives, which can be obtained by additional wave function evaluations and finite differences. A rotation trick can be used to reduce the number of additional locations at which the wave function must be evaluated [17].

A major problem arises in minimizing the variational energy for p -shell nuclei using the above wave functions: there is no variational minimum that gives reasonable rms radii. For example, the variational energy for ${}^6\text{Li}$ is slightly more bound than for ${}^4\text{He}$, but is not more bound than for separated ${}^4\text{He}$ and ${}^2\text{H}$ nuclei, so the wave function is not stable against breakup into $\alpha + d$ subclusters. Consequently, the energy can be lowered toward the sum of ${}^4\text{He}$ and ${}^2\text{H}$ energies by making the wave function more and more diffuse. Such a diffuse wave function would not be useful for computing other nuclear properties, or as a starting point for the GFMC calculation, so we constrain our search for optimal variational parameters by requiring the resulting point proton rms radius, r_p , to be close to the experimental values for ${}^6\text{Li}$ and ${}^7\text{Li}$ ground states. For other $A = 6 - 8$ ground states, and all the excited states, there are no experimental measurements of the charge radii. To avoid introducing too many additional parameter values, we construct these wave functions by making minimal changes to the ${}^6\text{Li}$ and ${}^7\text{Li}$ wave functions, with the added requirement that excited states should not have smaller radii than the ground states. The final step is always the diagonalization of the Hamiltonian in the $\beta_{LS[n]}$ mixing parameters.

4. GREEN'S FUNCTION MONTE CARLO

The GFMC method projects out the exact lowest-energy state, Ψ_0 , for a given set of quantum numbers, using $\Psi_0 = \lim_{\tau \rightarrow \infty} \exp[-(H - E_0)\tau]\Psi_T$, where Ψ_T is an initial trial function. The method used here is discussed in detail in Ref. [2]. The eigenvalue E_0 is calculated exactly while other expectation values are generally calculated neglecting terms of order $|\Psi_0 - \Psi_T|^2$ and higher. In contrast, the error in the variational energy, E_V , is of order $|\Psi_0 - \Psi_T|^2$, and other expectation values calculated with Ψ_T have errors of order $|\Psi_0 - \Psi_T|$.

We use the Ψ_T of Eq.(28) and define the propagated wave function $\Psi(\tau)$ as

$$\Psi(\tau) = e^{-(H-E_0)\tau} \Psi_T; \quad (37)$$

obviously $\Psi(\tau = 0) = \Psi_T$ and $\Psi(\tau \rightarrow \infty) = \Psi_0$. Introducing a small time step, $\Delta\tau$, $\tau = n\Delta\tau$, gives

$$\Psi(\tau) = \left[e^{-(H-E_0)\Delta\tau} \right]^n \Psi_T. \quad (38)$$

The $\Psi(\tau)$ is represented by a vector function of $\mathbf{R}$ using Eq.(35), and the Green's function, $G_{\alpha\beta}(\mathbf{R}, \mathbf{R}')$ is a matrix function of $\mathbf{R}$ and $\mathbf{R}'$ in spin-isospin space, defined as

$$G_{\alpha\beta}(\mathbf{R}, \mathbf{R}') = \langle \mathbf{R}, \alpha | e^{-(H-E_0)\Delta\tau} | \mathbf{R}', \beta \rangle. \quad (39)$$

It is calculated with leading errors of order $(\Delta\tau)^3$. Omitting spin-isospin indices for brevity, $\Psi(\mathbf{R}_n, \tau)$ is given by

$$\Psi(\mathbf{R}_n, \tau) = \int G(\mathbf{R}_n, \mathbf{R}_{n-1}) \cdots G(\mathbf{R}_1, \mathbf{R}_0) \Psi_T(\mathbf{R}_0) d\mathbf{R}_{n-1} \cdots \mathbf{R}_1 d\mathbf{R}_0. \quad (40)$$

The short-time propagator should allow as large a time step $\Delta\tau$ as possible, because the total computational time for propagation is proportional to $1/\Delta\tau$. Earlier calculations [1, 18, 19] used the propagator obtained from the Feynman formulae. Ignoring three-nucleon interaction terms in H , it is given by

$$e^{-H\Delta\tau} = \left[\mathcal{S} \prod_{i<j} e^{-v_{ij}\Delta\tau/2} \right] e^{-K\Delta\tau} \left[\mathcal{S} \prod_{i<j} e^{-v_{ij}\Delta\tau/2} \right] + \mathcal{O}(\Delta\tau^3). \quad (41)$$

Note that it is useful to symmetrize the product of $e^{-v_{ij}\Delta\tau/2}$ when $[v_{ij}, v_{jk}] \neq 0$, in order to reduce the error per iteration. The nuclear v_{ij} has a repulsive core of order GeV. The main error in the above propagator comes from terms in $e^{-H\Delta\tau}$ having multiple v_{ij} , like $v_{ij}Kv_{ij}(\Delta\tau)^3$, which can become large when particles i and j are very close. In order to make them negligible a rather small $\Delta\tau \sim 0.1 \text{ GeV}^{-1}$ is used with the above propagator. The matrix elements of the propagator are given by:

$$G_{\alpha\beta}(\mathbf{R}, \mathbf{R}') = G_0(\mathbf{R}, \mathbf{R}') \langle \alpha | \left[\mathcal{S} \prod_{i<j} e^{-v_{ij}(\mathbf{r}_{ij})\Delta\tau/2} \right] \left[\mathcal{S} \prod_{i<j} e^{-v_{ij}(\mathbf{r}'_{ij})\Delta\tau/2} \right] | \beta \rangle, \quad (42)$$

$$G_0(\mathbf{R}, \mathbf{R}') = \langle \mathbf{R} | e^{-K\Delta\tau} | \mathbf{R}' \rangle = \left[\sqrt{\frac{m}{2\pi\hbar^2\Delta\tau}} \right]^{3A} \exp \left[\frac{-(\mathbf{R} - \mathbf{R}')^2}{2\hbar^2\Delta\tau/m} \right]. \quad (43)$$

However, it has been found in studies of bulk helium atoms [20] that including the exact two-body propagator allows much larger time steps. This short-time propagator is

$$G_{\alpha\beta}(\mathbf{R}, \mathbf{R}') = G_0(\mathbf{R}, \mathbf{R}') \langle \alpha | \left[\mathcal{S} \prod_{i<j} \frac{g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})} \right] | \beta \rangle, \quad (44)$$

where g_{ij} is the exact two-body propagator,

$$g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}) = \langle \mathbf{r}_{ij} | e^{-H_{ij}\Delta\tau} | \mathbf{r}'_{ij} \rangle, \quad (45)$$

and $g_{0,ij}$ is the free two-body propagator. All terms containing any number of the same v_{ij} and K are treated exactly in this propagator, as we have included the imaginary-time equivalent of the full two-body scattering amplitude. It still has errors of order $(\Delta\tau)^3$, however they are from commutators of terms like $v_{ij}T v_{ik}(\Delta\tau)^3$ which become large only when both pairs ij and ik are close. Because this is a rare occurrence, a five times larger time step $\Delta\tau \sim 0.5 \text{ GeV}^{-1}$ can be used [2].

Including the three-body forces and the E_0 in Eq.(39), the complete propagator is given by

$$G_{\alpha\beta}(\mathbf{R}, \mathbf{R}') = e^{E_0\Delta\tau} G_0(\mathbf{R}, \mathbf{R}') \exp\left[-\sum (V_{ijk}^R(\mathbf{R}) + V_{ijk}^R(\mathbf{R}')) \frac{\Delta\tau}{2}\right] \\ \langle\alpha|I_3(\mathbf{R})|\gamma\rangle\langle\gamma|\left[\mathcal{S} \prod_{i<j} \frac{g_{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})}{g_{0,ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij})}\right]|\delta\rangle\langle\delta|I_3(\mathbf{R}')|\beta\rangle, \quad (46)$$

where

$$I_3(\mathbf{R}) = \left[1 - \frac{\Delta\tau}{2} \sum V_{ijk}^{2\pi}(\mathbf{R})\right]. \quad (47)$$

With the exponential of $V_{ijk}^{2\pi}$ expanded to first order in $\Delta\tau$, there are additional error terms of the form $V_{ijk}^{2\pi} V_{i'j'k'}^{2\pi} (\Delta\tau)^2$. However, they have negligible effect because $V_{ijk}^{2\pi}$ has a magnitude of only a few MeV.

The mixed expectation value of an operator O is defined as:

$$\langle O \rangle_{Mixed} = \frac{\langle \Psi_T | O | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle} \\ = \frac{\int d\mathbf{P}_n \Psi_T^\dagger(\mathbf{R}_n) O G(\mathbf{R}_n, \mathbf{R}_{n-1}) \cdots G(\mathbf{R}_1, \mathbf{R}_0) \Psi_T(\mathbf{R}_0)}{\int d\mathbf{P}_n \Psi_T^\dagger(\mathbf{R}_n) G(\mathbf{R}_n, \mathbf{R}_{n-1}) \cdots G(\mathbf{R}_1, \mathbf{R}_0) \Psi_T(\mathbf{R}_0)}, \quad (48)$$

where $\mathbf{P}_n = \mathbf{R}_0, \mathbf{R}_1, \dots, \mathbf{R}_n$ denotes the 'path', and $d\mathbf{P}_n = d\mathbf{R}_0 d\mathbf{R}_1 \cdots d\mathbf{R}_n$. In GFMC, the integral over the paths is carried out stochastically. Generally, the required expectation values are calculated approximately from the variational Ψ_T and mixed expectation values. Let

$$\Psi(\tau) = \Psi_T + \delta\Psi(\tau). \quad (49)$$

Retaining only the terms of order $\delta\Psi(\tau)$, we obtain

$$\langle O(\tau) \rangle = \frac{\langle \Psi(\tau) | O | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}, \approx \langle O(\tau) \rangle_{Mixed} + [\langle O(\tau) \rangle_{Mixed} - \langle O \rangle_T],$$

where

$$\langle O \rangle_T = \frac{\langle \Psi_T | O | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}. \quad (50)$$

More accurate evaluations of $\langle O(\tau) \rangle$ are possible [21], essentially by measuring the observable at the mid-point of the path. However, such estimates require a propagation

twice as long as the mixed estimate. Because we are limited in the present calculations to a total propagation time of 0.06 MeV^{-1} , we use the approximation (50).

An important exception to the above is the energy, E_0 given by $\langle H(\tau \rightarrow \infty) \rangle$. The $\langle H(\tau) \rangle_{Mixed}$ can be re-expressed as [22]

$$\langle H(\tau) \rangle_{Mixed} = \frac{\langle \Psi_T | e^{-(H-E_0)\tau/2} H e^{-(H-E_0)\tau/2} | \Psi_T \rangle}{\langle \Psi_T | e^{-(H-E_0)\tau/2} e^{-(H-E_0)\tau/2} | \Psi_T \rangle}, \quad (51)$$

since the propagator $\exp[-(H-E_0)\tau]$ commutes with the Hamiltonian. Thus $\langle H(\tau) \rangle_{Mixed}$ approaches E_0 in the limit $\tau \rightarrow \infty$, and furthermore, being an expectation value of H , it obeys the variational principle

$$\langle H(\tau) \rangle_{Mixed} \geq E_0. \quad (52)$$

Terms in the Hamiltonian which involve the square of the momentum operator introduce large statistical errors, as discussed in Ref. [2]. Hence, the GFMC propagator is actually constructed with the simpler H' given in Eq.(17). Consequently, the upper bound property applies to $\langle H'(\tau) \rangle$, and $\langle H - H' \rangle$ must be evaluated using Eq.(50).

The construction of the short-time propagator and the method for sampling the paths are discussed in detail in Ref. [2]. One major complication that arises in the algorithm is the 'fermion sign problem'. Wave functions of simple Fermi systems have domains of positive and negative signs separated by nodal surfaces.

Figure 1. GFMC transient energy for ${}^6\text{Li}$

When the path $\mathbf{P}$ crosses a nodal surface, the variance of the mixed expectation value starts to increase. This seldom happens for small time steps, but as τ increases, this noise builds up and it effectively limits the value of τ to 0.06 MeV^{-1} for most of the nuclei studied here. The problem is exacerbated if one has a poor starting trial function Ψ_T .

The progress of a GFMC calculation is illustrated in Fig. 1, where $E(\tau)$ for ${}^6\text{Li}$ is plotted. The GFMC energies are shown by points with error bars; it can be seen that the error grows with increasing τ . Most of our calculations are made up to $\tau = 0.06 \text{ MeV}^{-1}$, but in this case they were pushed to $\tau = 0.10 \text{ MeV}^{-1}$. The curves shown are attempts to extrapolate $E(\tau)$ with a sum of exponentially decaying excited states; we conclude it is safest to simply take the average of the last few points (usually $\tau=0.04\text{--}0.06 \text{ MeV}^{-1}$) as the final GFMC energy. As discussed in Ref. [2], we believe these averages are reliable upper bounds to the eigenenergies of H , and are probably within $\sim 0.3 \text{ MeV}$ of the exact energy for $A = 6$, and $\sim 0.5 \text{ MeV}$ for $A = 7$.

We performed a number of tests with different Ψ_T as starting points for the GFMC calculation [2]. We found the most crucial aspect in choosing Ψ_T is that it have the correct mix of spatial symmetries, i.e., the $\beta_{LS[n]}$ admixtures. This is because the limited propagation time is not sufficient for the GFMC algorithm to filter out low-lying excitations with the same quantum numbers. This issue is unimportant in ${}^4\text{He}$, where the first 0^+ excited state is near 20 MeV , but in ${}^6\text{Li}$, the first 1^+ excited state is only 5.65 MeV ; other p -shell nuclei have similar low-lying excitations. Otherwise, the GFMC algorithm is able to rapidly correct for some very poor Ψ_T whose variational energies are actually positive. However, a good Ψ_T helps to keep the error bars small at larger τ . The most efficient balance between speed of construction of Ψ_T and smallest number of samples needed to achieve a given error bar is given by Eq.(28). A number of other tests of the GFMC algorithm and its ability to determine nuclear radii are described in Ref. [2].

The calculations described here are computationally intense, and would not have been possible without the advent of parallel supercomputers. Our initial studies of ${}^6\text{Li}$ [1] required ~ 2000 node hours on an IBM SP1 to propagate 10,000 configurations to $\tau = 0.06 \text{ MeV}^{-1}$. Today, with improvements in the algorithm and after much effort to optimize the computer codes, the same calculation requires only 20 node hours on the next generation machine, an IBM SP2. However, a present calculation for ${}^8\text{He}$, requiring 50,000 configurations to get a reasonable error bar, takes 3,000 SP2 node hours, so forefront computer resources remain essential for this program.

5. ENERGY RESULTS

The chief results of this work are the ground and excited state energies shown in Fig. 2 and tabulated in Tables 2 and 4. The results for $A = 6, 7$ have been reported previously [2]; the results for $A = 8$ are preliminary. The VMC calculations using Ψ_T , the simpler trial function that serves as the GFMC starting point, are 4-5% above the final GFMC ground state results for $A = 3 - 4$ nuclei, the latter having been fit to the experimental energies by construction of V_{ijk} . The more sophisticated Ψ_V gets within 2% of the exact $A = 3 - 4$ energies. However, the variational calculations get progressively worse for $A = 4 - 6$, with Ψ_T being 13-17% above the final GFMC results, and Ψ_V at 10-12% above, for nuclei with $N \sim Z$.

Figure 2. Experimental and calculated energy spectrum

Table 2

Experimental and quantum Monte Carlo energies of $A=2-8$ nuclear ground states in MeV.

${}^A Z(J^\pi; T)$	VMC (Ψ_T)	VMC (Ψ_V)	GFMC	Expt.
${}^2\text{H}(1^+; 0)$	-2.2248(5)			-2.2246
${}^3\text{H}(\frac{1}{2}^+; \frac{1}{2})$	-8.15(1)	-8.32(1)	-8.47(1)	-8.48
${}^4\text{He}(0^+; 0)$	-26.93(2)	-27.78(3)	-28.30(2)	-28.30
${}^6\text{He}(0^+; 1)$	-23.77(6)	-24.87(7)	-27.64(14)	-29.27
${}^6\text{Li}(1^+; 0)$	-27.04(3)	-28.09(7)	-31.25(11)	-31.99
${}^7\text{He}(\frac{3}{2}^-; \frac{3}{2})$	-19.02(8)	-20.43(12)	-25.16(16)	-28.82
${}^7\text{Li}(\frac{3}{2}^-; \frac{1}{2})$	-31.59(8)	-32.78(11)	-37.44(28)	-39.24
${}^8\text{He}(0^+; 2)$	-17.03(14)	-19.71(18)	-25.77(61)	-31.41
${}^8\text{Li}(2^+; 1)$	-27.59(16)	-29.70(19)	-38.26(19)	-41.28
${}^8\text{Be}(0^+; 0)$	-45.63(17)	-48.06(27)	-54.66(64)	-56.50

In absolute terms, Ψ_V misses about 1.5 MeV of additional binding for each p -shell nucleon that is added. Clearly, there is some significant feature of light p -shell nuclei that we do not yet know how to model in our trial functions.

We also observe that the GFMC results are underbound compared to experiment. The Li isotopes are stable against breakup into subclusters, but progressively more underbound as A increases. This is probably a failure of our interaction model. There is also an isospin problem with our interaction, in that the He isotopes are even further off from the experimental values, and in fact do not show stability against breakup into subclusters.

A detailed breakdown of the GFMC interaction energy into kinetic, two- and three-nucleon interactions is given in Table 3. Because of the mixed expectation values these components are not as accurate as the total energy, and do not quite add up to the full amount. Nevertheless, they give a good idea about the relative size of the different terms involved. We observe that there is a big cancellation between the kinetic and two-body potential terms. Consequently, while V_{ijk} is less than 5% of v_{ij} in magnitude, it

Table 3

Kinetic and potential energy contributions to GFMC energies in MeV.

${}^A Z(J^\pi; T)$	K	v_{ij}	V_{ijk}	v_{ij}^γ	v_{ij}^π	$V_{ijk}^{2\pi}$
${}^2\text{H}(1^+; 0)$	19.81	-22.04	0.0	0.018	-21.28	0.0
${}^3\text{H}(\frac{1}{2}^+; \frac{1}{2})$	50.8(5)	-58.4(5)	-1.20(2)	0.04	-43.8(2)	-2.17(1)
${}^4\text{He}(0^+; 0)$	111.9(6)	-135.4(6)	-6.4(1)	0.86	-99.4(2)	-11.7(1)
${}^6\text{He}(0^+; 1)$	140.3(15)	-165.0(15)	-7.2(2)	0.87(1)	-109.0(4)	-13.6(2)
${}^6\text{Li}(1^+; 0)$	150.8(10)	-179.2(10)	-7.2(1)	1.71(1)	-128.9(5)	-13.5(1)
${}^7\text{He}(\frac{3}{2}^-; \frac{3}{2})$	146.0(17)	-170.4(17)	-7.4(2)	0.86(1)	-109.9(6)	-14.1(2)
${}^7\text{Li}(\frac{3}{2}^-; \frac{1}{2})$	186.4(28)	-220.8(30)	-8.9(2)	1.78(2)	-152.5(7)	-17.1(4)
${}^8\text{He}(0^+; 2)$	169.1(54)	-195.4(57)	-8.3(5)	0.87(2)	-121.1(9)	-15.8(8)
${}^8\text{Li}(2^+; 1)$	223.2(22)	-261.0(21)	-11.2(2)	1.88(1)	-156.6(9)	-22.2(3)
${}^8\text{Be}(0^+; 0)$	246.3(56)	-295.8(62)	-14.8(5)	3.39(6)	-224.1(9)	-28.1(8)

contributes up to 25% of the net binding. Among the subcomponents of v_{ij} , the one-pion exchange dominates, particularly for $N = Z$ nuclei. Similarly, the two-pion exchange is the dominant component of V_{ijk} . We also note that the shorter-range V_{ijk}^R (which is not shown but can be obtained by subtraction) is much larger than the discrepancy between the total GFMC energy and experiment. Thus we may reasonably hope that improvements in our modelling of this phenomenology will make it possible to reproduce the observed energies. Finally, we note that the electromagnetic v_{ij}^γ is dominated by the Coulomb interaction between protons, $V_{C1}(pp)$, but about 17% (8%) of its total contribution comes from the magnetic moment and other terms in Eqs.(4-6) in He (Li) isotopes.

Table 4

Experimental, VMC, and GFMC excitation energies (adjusted to their respective ground states) in MeV.

$AZ(J^\pi; T)$	Expt.	VMC	GFMC
${}^6\text{He}(2^+; 1)$	1.80	1.86(10)	1.80(18)
${}^6\text{He}(1^+; 1)$		3.46(10)	
${}^6\text{He}(2^+; 1)$		3.61(10)	
${}^6\text{He}(0^+; 1)$		5.24(11)	
${}^6\text{Li}(3^+; 0)$	2.19	2.93(10)	2.72(36)
${}^6\text{Li}(0^+; 1)$	3.56	3.84(10)	3.94(23)
${}^6\text{Li}(2^+; 0)$	4.31	4.23(11)	4.43(39)
${}^6\text{Li}(2^+; 1)$	5.37	5.64(10)	
${}^6\text{Li}(1^+; 0)$	5.65	5.68(11)	
${}^6\text{Li}(1^+; 0)$		8.96(11)	
${}^7\text{He}(\frac{1}{2}^-; \frac{3}{2})$		0.90(16)	
${}^7\text{He}(\frac{5}{2}^-; \frac{3}{2})$		1.69(16)	
${}^7\text{He}(\frac{3}{2}^-; \frac{3}{2})$		2.08(16)	
${}^7\text{Li}(\frac{1}{2}^-; \frac{1}{2})$	0.48	0.33(16)	0.76(41)
${}^7\text{Li}(\frac{7}{2}^-; \frac{1}{2})$	4.63	5.48(16)	5.72(41)
${}^7\text{Li}(\frac{5}{2}^-; \frac{1}{2})$	6.68	6.64(16)	6.56(45)
${}^7\text{Li}(\frac{5}{2}^-; \frac{1}{2})$	7.46	9.90(16)	
${}^7\text{Li}(\frac{7}{2}^-; \frac{1}{2})$	9.67	11.63(16)	
${}^7\text{Li}(\frac{3}{2}^-; \frac{1}{2})$	9.90	10.14(16)	
${}^7\text{Li}(\frac{1}{2}^-; \frac{1}{2})$		10.79(16)	
${}^7\text{Li}(\frac{3}{2}^-; \frac{3}{2})$	11.24	13.05(16)	12.65(33)
${}^8\text{He}(2^+; 2)$	2.6	2.34(25)	
${}^8\text{Li}(1^+; 1)$	0.98	1.19(26)	
${}^8\text{Li}(3^+; 1)$	2.26	2.81(25)	
${}^8\text{Li}(4^+; 1)$	6.53	5.63(26)	
${}^8\text{Be}(2^+; 0)$	3.04	3.90(37)	
${}^8\text{Be}(4^+; 0)$	11.4	11.96(35)	

Despite the difficulties with the ground state energies, the VMC and GFMC calculations give a reasonable description of the excitation spectra for the $A = 6 - 8$ nuclei, as seen in Table 4. We have calculated eight excited states using both VMC and GFMC, and find good agreement with each other and with experiment. An additional 19 states have been calculated with VMC alone, making use of the direct diagonalizations to predict multiple states with the same quantum numbers. In particular, the first excited $(1^+;0)$ state in ${}^6\text{Li}$ and the first excited $(\frac{3}{2}^-; \frac{1}{2})$ state in ${}^7\text{Li}$ are very close to their experimental values. We also predict a number of states in ${}^6\text{He}$ and ${}^7\text{He}$ which have not been observed, but which could be searched for. While we generally have the correct ordering of states, the spin-orbit splittings within multiplets is often too small; for example, the weak splitting of the ${}^3\text{D}_{1,2,3}$ multiplet in ${}^6\text{Li}$ results in a $(3^+;0)$ energy that is too high with respect to the ground state.

We have also calculated all the states in Be, B, and C that are isobaric analogs to those discussed above using VMC, and some with GFMC. Energy differences among these states are sensitive probes of the charge-independence-breaking parts of the Hamiltonian. The energies for a given isomultiplet of states can be expanded as

$$E_{A,T}(T_z) = \sum_{n \leq 2T} a_n(A, T) Q_n(T, T_z), \quad (53)$$

where $Q_0 = 1$, $Q_1 = T_z$, and $Q_2 = \frac{1}{2}(3T_z^2 - T^2)$ are isoscalar, isovector, and isotensor terms [23]. The isovector and isotensor coefficients $a_n(A, T)$ calculated in VMC are given in Table 5. Where GFMC coefficients have been calculated, they are in fair agreement.

The charge-symmetry-breaking in the $A = 3$ nuclei is well-explained with the current model, but for p -shell nuclei the isovector coefficients are underestimated with increasing A and/or T , while mixed results are obtained for the isotensors. However, the significant underbinding with the present Hamiltonian as A and T increase may mean that our wave functions are too diffuse; the contraction obtained with correct binding would increase both the dominant electromagnetic terms and the short-range CSB contribution and would improve the isovector coefficients.

Table 5

VMC isovector and isotensor energy coefficients $a_n(A, T)$ in MeV.

$a_n(A, T)$	K_{CSB}	v^γ	v^{CSB}	v^{CD}	Total	Expt.
$a_1(3, \frac{1}{2})$	0.014	0.680(1)	0.066	0.	0.760(1)	0.764
$a_1(6, 1)$	0.014	1.048(2)	0.035(1)	0.	1.097(3)	1.173
$a_2(6, 1)$	0.	0.186(1)	0.	0.101(12)	0.287(12)	0.223
$a_1(7, \frac{1}{2})$	0.025	1.501(3)	0.080(1)	0.	1.605(4)	1.644
$a_1(7, \frac{3}{2})$	0.011	1.109(4)	0.021(2)	0.	1.141(5)	1.373
$a_2(7, \frac{3}{2})$	0.	0.119(1)	0.	0.020(4)	0.139(4)	0.175
$a_1(8, 1)$	0.019	1.559(8)	0.049(1)	0.	1.628(5)	1.770
$a_1(8, 2)$	0.014	1.371(5)	0.031(1)	0.	1.416(6)	1.659
$a_2(8, 2)$	0.	0.127(3)	0.	0.017(5)	0.144(7)	0.153

6. DENSITY AND MOMENTUM DISTRIBUTIONS

In addition to the energies, we have calculated a variety of one- and two-nucleon density distributions, momentum distributions, and electromagnetic properties. The proton rms radii and static electromagnetic properties are given in Table 6. These are calculated from Ψ_V using impulse approximation. In general, we know that there are significant corrections to the electromagnetic moments from two-body charge and current contributions [24,25]. For the magnetic moments, these corrections are only ~ 1 -2% in isoscalar nuclei like ^2H , but are ~ 15 -20% in the isovector $T = \frac{1}{2}$ nuclei ^3H and ^3He . Therefore it is not surprising that we see very little discrepancy for the magnetic moment in ^6Li , but sizeable errors for ^7Li , ^8Li , and ^8B . Presumably, calculations including meson-exchange contributions would come much closer to the experimental values in the latter cases.

Table 6

VMC values for proton rms radii (in fm), for magnetic moments (in μ_N), and quadrupole moments (in fm^2) in impulse approximation.

	$\langle r_p^2 \rangle^{1/2}$		μ		Q	
	VMC	Expt.	VMC	Expt.	VMC	Expt.
$^2\text{H}(1^+; 0)$	1.967	1.953	0.847	0.857	0.270	0.286
$^3\text{H}(\frac{1}{2}^+; \frac{1}{2})$	1.59(1)	1.60	2.582(1)	2.979		
$^3\text{He}(\frac{1}{2}^+; \frac{1}{2})$	1.74(1)	1.77	-1.770(1)	-2.128		
$^4\text{He}(0^+; 0)$	1.47(1)	1.47				
$^6\text{He}(0^+; 1)$	1.95(1)					
$^6\text{Li}(1^+; 0)$	2.46(2)	2.43	0.828(1)	0.822	-0.33(18)	-0.083
$^6\text{Be}(0^+; 1)$	2.96(4)					
$^7\text{Li}(\frac{3}{2}^-; \frac{1}{2})$	2.26(1)	2.27	2.924(2)	3.256	-3.31(29)	-4.06
$^7\text{Be}(\frac{3}{2}^-; \frac{1}{2})$	2.42(1)		-1.110(2)		-5.64(45)	
$^8\text{He}(0^+; 2)$	1.93(2)					
$^8\text{Li}(2^+; 1)$	2.31(2)		0.976(5)	1.653	3.32(37)	3.11(5)
$^8\text{Be}(0^+; 0)$	2.29(2)					
$^8\text{B}(2^+; 1)$	2.66(3)		1.672(6)	1.036	7.08(71)	6.83(21)
$^8\text{C}(0^+; 2)$	3.12(5)					

The small quadrupole moment of ^6Li is a difficult problem, where there is a delicate cancellation between the contributions from the deuteron quadrupole moment and the D -wave part of the α - d relative wave function. Many cluster models for ^6Li fail to obtain the observed negative sign; we have trouble getting a small enough magnitude. In the case of ^7Li , where there is no such delicate cancellation, the value is only ~ 15 -20% too low in magnitude, while the ^8Li and ^8B values are surprisingly good.

In Fig. 3 we give the proton and neutron spin densities in ^6Li , which may be of use in the characterization of spin-polarized ^6LiD as an effective polarized neutron target. The integrated neutron densities are found to be 1.93 for spin up and 1.09 for spin down, respectively, yielding a net polarization of 29% [2].

Figure 3. Spin polarization densities for ${}^6\text{Li}$

Figure 4. Momentum distributions for ${}^6\text{Li}$

The proton momentum distribution, $N_p(k)$, in ${}^6\text{Li}$ is shown in Fig. 4 along with the αd overlap, $N_{\alpha d}$. These are the result of improved versions of the calculations described in Refs. [26,27]. Integration over k gives three protons in ${}^6\text{Li}$ as it should, while the αd spectroscopic factor is 0.86.

Preliminary VMC calculations of elastic and inelastic electromagnetic form factors for ${}^6\text{Li}$ are shown in Fig. 5. These have been made in impulse approximation (IA) and with meson-exchange contributions (MEC) to the charge and density operators. The comparison with data for the elastic longitudinal form factor, $F_L(q^2)$, is excellent, as is the E2 transition to the 3^+ first excited state. The MEC corrections are small, but stand out noticeably in the first minimum where they significantly improve the fit to data. The M1 transition to the 0^+ isobaric analog state is also reproduced reasonably well. The elastic transverse form factor, $F_T(q^2)$, is good up to the first zero, but then is too large in the region of the second maximum. We plan to repeat these studies with the GFMC wave function to see if the present deficiencies can be removed. Nevertheless, these calculations, which have been done without effective charges as commonly needed in shell-model studies, give a remarkably good explanation of the electron scattering data.

7. CONCLUSIONS AND OUTLOOK

Quantum Monte Carlo methods can now be used to obtain accurate (within 1%) energies for light p -shell nuclei up to $A = 8$. This has been made possible by the rapid growth of computational power, due to parallel supercomputers, and a continuing evolution of algorithms, often inspired by work in condensed matter physics. With these calculations, we can see for the first time the nuclear shell structure emerging directly from bare NN interactions that fit two-body scattering data.

The future of QMC calculations in light nuclei is very promising. A new algorithm, called ‘constrained path’ GFMC, promises a significant reduction in the fermion sign noise and the ability to propagate to larger Euclidean time τ [28]. The present method should be extensible to slightly larger nuclei with the next generation of computers, e.g., ${}^9\text{Be}$ (${}^{10}\text{He}$) should be about 3 (5) times more expensive to compute than ${}^8\text{Li}$. For larger nuclei, we are working on a fusion of the cluster VMC methods [29] that have been used in ${}^{16}\text{O}$, and the GFMC algorithm.

A major effort is now underway to improve the Hamiltonian to fit the observed $A = 6-8$ spectrum at the 1% level. Additions include the relativistic “boost” correction [8,9] that is about $\sim 35\%$ of V_{ijk}^R in ${}^3\text{H}$ and ${}^4\text{He}$. We are also examining a three-nucleon spin-orbit force, which significantly improves the spin-orbit splittings in $A = 6-7$ nuclei, and may help to solve the A_y puzzle in Nd scattering [30]. Other possible short-range V_{ijk} may be related to (and constrained by) the threshold pion production in NN scattering [7].

There are also many astrophysical applications for the $A = 6-8$ nuclear wave functions, such as the radiative captures ${}^4\text{He}(d, \gamma){}^6\text{Li}$, for primordial nucleosynthesis, and ${}^7\text{Be}(p, \gamma){}^8\text{B}$ for the solar neutrino problem. QMC methods are also being used to study neutron “drops”, finite systems of neutrons in an external potential well, that can be used as a development tool for Skyrme interactions [31], with applications in neutron-rich nuclei like those found in the crusts of neutron stars.

We expect many new results by FBXVI!

Figure 5. Calculated elastic and transition form factors in ${}^6\text{Li}$

8. ACKNOWLEDGMENTS

It is a pleasure to thank my colleagues Ana Arriaga, Joe Carlson, Jun Forest, Vijay Pandharipande, Steve Pieper, Brian Pudliner, Rocco Schiavilla, and Vincent Stoks for their contributions to this work. The calculations described here were made possible by generous grants of time from the Mathematical and Computer Science Division of Argonne National Laboratory, and the Cornell Theory Center.

REFERENCES

1. B. S. Pudliner, V. R. Pandharipande, J. Carlson, and R. B. Wiringa, Phys. Rev. Lett. **74**, 4396 (1995).
2. B. S. Pudliner, V. R. Pandharipande, J. Carlson, S. C. Pieper, and R. B. Wiringa, Phys. Rev. C **56**, in press (1997).
3. R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
4. J. R. Bergervoet, P. C. van Campen, R. A. M. Klomp, J.-L. de Kok, T. A. Rijken, V. G. J. Stoks, and J. J. de Swart, Phys. Rev. C **41**, 1435 (1990).
5. V. G. J. Stoks, R. A. M. Klomp, M. C. M. Rentmeester, and J. J. de Swart, Phys. Rev. C **48**, 792 (1993).
6. J. Fujita and H. Miyazawa, Prog. Theor. Phys. **17**, 360 (1957).
7. S. A. Coon, M. T. Peña, and D. O. Riska, Phys. Rev. C **52**, 2925 (1995).
8. J. L. Forest, V. R. Pandharipande, and J. L. Friar, Phys. Rev. C **52**, 568 (1995).
9. J. L. Forest, V. R. Pandharipande, J. Carlson, and R. Schiavilla, Phys. Rev. C **52**, 576 (1995).
10. R. B. Wiringa, Rev. Mod. Phys. **65**, 231 (1993).
11. A. Arriaga, V. R. Pandharipande, and R. B. Wiringa, Phys. Rev. C **52**, 2362 (1995).
12. R. B. Wiringa, Phys. Rev. C **43**, 1585 (1991).
13. S. Cohen and D. Kurath, Nucl. Phys. **73**, 1 (1965); Nucl. Phys. **A101**, 1 (1967).
14. A. Bohr and B. R. Mottelson, *Nuclear Structure Volume I*, (W. A. Benjamin, New York, 1969).
15. J. A. Carlson and R. B. Wiringa, in *Computational Nuclear Physics 1*, edited by K. Langanke, J. A. Maruhn, and S. E. Koonin (Springer Verlag, Berlin, 1991).
16. B. S. Pudliner, Ph.D. thesis, University of Illinois (1996).
17. R. Schiavilla, V. R. Pandharipande, and A. Fabrocini, Phys. Rev. C **40**, 1484 (1989).
18. J. Carlson, Phys. Rev. C **36**, 2026 (1987).
19. J. Carlson, Phys. Rev. C **38**, 1879 (1988).
20. D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).
21. M. H. Kalos, J. Comp. Phys. **2**, 257 (1967).
22. D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Heidelberg, 1979).
23. M. Peshkin, Phys. Rev. **121**, 636 (1960).
24. R. Schiavilla, V. R. Pandharipande, and D. O. Riska, Phys. Rev. C **40**, 2294 (1989).
25. R. Schiavilla, V. R. Pandharipande, and D. O. Riska, Phys. Rev. C **41**, 309 (1990).
26. R. Schiavilla, V. R. Pandharipande, and R. B. Wiringa, Nucl. Phys. **A449**, 219 (1986).
27. J. L. Forest, V. R. Pandharipande, S. C. Pieper, R. B. Wiringa, R. Schiavilla, and A. Arriaga, Phys. Rev. C **54**, 646 (1996).
28. Shiwei Zhang, J. Carlson, and J. E. Gubernatis, Phys. Rev. Lett. **74**, 3653 (1995).
29. S. C. Pieper, R. B. Wiringa, and V. R. Pandharipande, Phys. Rev. C **46**, 1741 (1992).
30. H. Witala, D. Hüber, and W. Glöckle, Phys. Rev. C **49**, R14 (1994).
31. B. S. Pudliner, A. Smerzi, J. Carlson, V. R. Pandharipande, S. C. Pieper, and D. G. Ravenhall, Phys. Rev. Lett. **76**, 2416 (1996).