Quantum Monte Carlo Calculations of $A \leq 6$ Nuclei

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Abstract

The energies of $^3H$, $^3He$, and $^4He$ ground states, the $\frac{3}{2}^-$ and $\frac{1}{2}^-$ scattering states of $^5He$, the ground states of $^6He$, $^6Li$, and $^6Be$ and the $3^+$ and $0^+$ excited states of $^6Li$ have been accurately calculated with the Green’s function Monte Carlo method using realistic models of two- and three-nucleon interactions. The splitting of the $A = 3$ isospin $T = \frac{1}{2}$ and $A = 6$ isospin $T = 1$, $J^\pi = 0^+$ multiplets is also studied. The observed energies and radii are generally well reproduced, however, some definite differences between theory and experiment can be identified.
A system of interacting nonrelativistic nucleons is the simplest model of nuclei. Even in this simple model exact calculations have been possible only for a limited number of light nuclei due to the strong spin-isospin dependence of nuclear forces. For many years, only two-nucleon states could be exactly calculated. Next, the Faddeev method was used to study the three-nucleon states \[1,2\]. In the past decade, many advances have become possible due to the development of supercomputers. Quantum Monte Carlo methods were used to study nuclei with \( A \leq 5 \) \[3,4\], the \(^4\)He ground state was calculated with the Faddeev-Yakubovosky method \[5\], and methods using hyperspherical functions were developed to study low-energy three- and four-nucleon states \[6\]. In this letter, we report the first realistic six-nucleon (6N) quantum Monte Carlo calculations along with updated results for nuclei with \( A \leq 5 \). Until now the \( A = 6 \) nuclei have been mostly treated as three-body systems with an \( \alpha \) and two nucleons \[7\].

The new Argonne \( v_{18} \) two-nucleon interaction \[8\] is used here. It is expressed as a sum of four parts:

\[
v = v_{14} + v_{cib} + v_{csb} + v_{em}.
\]  

(1)

Its dominant part, \( v_{14} \), contains 14 isoscalar operators as in the old Argonne \( v_{14} \) \[9\]. The charge-independence-breaking part, \( v_{cib} \), has three isotensor terms with operators \([3\tau_i \cdot \tau_j - \tau_i \cdot \sigma_j - \tau_j \cdot \sigma_i] \otimes [1, \sigma_i \cdot \sigma_j, S_{ij}]\), and includes the effect of the mass difference between charged and neutral pions. The \( v_{cib} = 0 \) in isospin \( T = 0 \) states, while in \( T = 1 \) states \( v_{cib}(np) = -2v_{cib}(nn) = -2v_{cib}(pp) \). The isovector charge-symmetry-breaking part, \( v_{csb} \), contains the operator \((\tau_i \cdot \sigma_j + \tau_j \cdot \sigma_i)\); it accounts for the difference between \( nn \) and \( pp \) interactions and vanishes in \( np \) pairs. The electromagnetic part, \( v_{em} \), contains \( pp \) and \( np \) Coulomb and magnetic interactions in all pairs. The kinetic energy operator associated with this model has isoscalar and isovector parts denoted by \( K \) and \( K_{csb} \):

\[
K + K_{csb} = -\frac{\hbar^2}{4} \sum_i \left[ \left( \frac{1}{m_p} + \frac{1}{m_n} \right) \nabla_i^2 + \left( \frac{1}{m_p} - \frac{1}{m_n} \right) \tau \cdot \sigma_i \nabla_i^2 \right]
\]  

(2)
Due to its careful treatment of isospin-symmetry-breaking terms, the new Argonne \( v_{18} \) model is well-suited to study the mass differences between the \( T = \frac{1}{2}, 3^H e - 3^H H \) doublet and the \( T = 1, J^\pi = 0^+, 6^H e - 6^H Li - 6^H Be \) triplet.

Three-nucleon interactions, \( V_{ijk} \), described with the Urbana model \[10\] are included in the nuclear Hamiltonian. These contain a two-pion exchange part with its strength \( A_{2\pi} \) chosen to reproduce the observed binding energies of \( 3^H H \) and \( 4^H e \), and a phenomenological spin-isospin independent interaction of strength \( U_0 \) adjusted to obtain the empirical equilibrium density of nuclear matter. In Urbana models IX (VIII) of \( V_{ijk} \), to be used in conjunction with the new \( v_{18} \) (old \( v_{14} \)), these parameters have values \( A_{2\pi} = -0.0293 \) (−0.028) and \( U_0 = 0.0048 \) (0.005) MeV.

The Green’s function Monte Carlo (GFMC) calculations \[3,4\] are carried out with a simpler isoscalar Hamiltonian:

\[
\hat{H} = K + \sum_{i<j} v_8(ij) + \sum_{i<j<k} V_{ijk}. 
\]  

The interaction \( v_8(ij) \) has eight terms, with operators \([1, \tau_i \cdot \tau_j] \otimes [1, \sigma_i \cdot \sigma_j, S_{ij}, L \cdot S]\), chosen such that it equals the \( v_{14} \) in all \( S \)- and \( P \)-waves as well as in the \( 3^D_1 \) wave and its coupling to the \( 3^S_1 \). The eigenstates of \( \hat{H} \) are computed, and all other terms, namely \((v_{14} - v_8), v_{cib}, v_{csb}, v_{em}, \) and \( K_{csb} \), are treated as first order perturbations. The error in the binding energy of \( ^3H \) due to the perturbative treatment of \( v_{14} - v_8 \) has been estimated by Kamada and Glöckle \[11\] to be \( \sim 0.02 \) MeV.

Nuclear states are represented by vector functions \( \Psi(R) \) whose components \( \psi_\alpha(R) \) give the amplitudes for the nucleons, at spatial coordinates \( R = (r_1, r_2, \ldots, r_A) \), to be in spin-isospin state \( |\alpha\rangle \). The GFMC calculation of the lowest energy state with quantum numbers \( \xi(J^\pi, T, T_z) \) starts with an approximate wave function \( \Psi_v(R) \) determined from a variational Monte Carlo (VMC) calculation for that state. It yields values of \( \Psi(\tau, R_i(\tau)) \), where

\[
\Psi(\tau, R) = e^{-\hat{H} \tau} \Psi_v(R), \tag{4}
\]

at configurations \( R_i(\tau) \) distributed with probability \( |\Psi^\dagger_v(R) \Psi(\tau, R)| \). Here \( i \) labels configurations which number \( \sim 10,000 \). The \( e^{-\hat{H} \tau} \) is considered as a product of many small imaginary
time steps $e^{-\hat{H}\Delta\tau}$, with $\Delta\tau \sim 0.0001\,MeV^{-1}$. Using the small-time limit of the propagator $e^{-\hat{H}\Delta\tau}$, correct up to order $\Delta\tau$, the $\Psi(\tau + \Delta\tau, \mathbf{R}_i(\tau + \Delta\tau))$ are stochastically estimated from the known $\Psi(\tau, \mathbf{R}_i(\tau))$.

The number of spin-isospin states that contribute to the $T = 0(1)$ 6N $\Psi(\mathbf{R})$ is 320(576), and their propagator $e^{-\hat{H}\Delta\tau}$ is a $320 \times 320(576 \times 576)$ complex matrix function. Therefore 6N GFMC calculations are numerically very intensive. They were performed on the IBM SP parallel computer at Argonne National Laboratory with 128 nodes operating at $\sim 40$ MFLOPS/node. Propagating 10,000 6N configurations up to $\tau = 0.06\,MeV^{-1}$ requires $\sim 2,000$ node hours. In contrast, the $^4He$ ground state wave function $\Psi(\mathbf{R})$ has only 32 spin-isospin states, and requires $\sim 100$ node hours for a similar calculation.

It is well known that there are no $A = 5$ bound states. The $\frac{3}{2}^-$ and $\frac{1}{2}^-$ resonances in $^5He$ have been studied as $n - ^4He$ scattering and the phase shifts in these partial waves have been extracted [12]. The GFMC calculations for these states are carried out with an external $\alpha - n$ potential that vanishes for $|\mathbf{r}_\alpha - \mathbf{r}_n| < 12.5$ fm and is infinitely repulsive for $|\mathbf{r}_\alpha - \mathbf{r}_n| > 12.5$ fm. These conditions also imply that the external potential is $0(\infty)$ for $|\mathbf{r}_n| < 10(> 10)$ fm in the center of mass frame. The calculated $\Psi_o$ corresponds to a scattering solution with a node at $|\mathbf{r}_\alpha - \mathbf{r}_n| = 12.5$ fm, however, only the interesting part with $|\mathbf{r}_\alpha - \mathbf{r}_n| < 12.5$ fm is retained in the calculation. Assuming that the interaction between $\alpha$ and $n$ is negligible for $|\mathbf{r}_\alpha - \mathbf{r}_n| > 12.5$ fm the true energy of this state can be obtained from the phase shifts [13].

The variational wave functions used in these calculations include spatial and spin-isospin two-body and three-body correlations denoted by $f_c(r_{ij}), U_{ij}$, and $U_{ijk}$ in ref. [14]. The uncorrelated wave functions for $^3H$ and $^4He$ are as given in [14], while those for $^5He$ have an additional nucleon in the $(p_{\frac{3}{2}})$ or $(p_{\frac{1}{2}})$ scattering state. The two extra nucleons in 6N states are in optimized superpositions of $(p_{\frac{3}{2}})^2$, $(p_{\frac{1}{2}}p_{\frac{3}{2}})$, and $(p_{\frac{3}{2}})^2$ states whose radii are constrained to reasonable values. Details of the VMC and GFMC calculations will be published separately.
The transient energy $E(\tau)$ defined as:

$$E(\tau) = \frac{\langle \Psi_v | \hat{H} | \Psi(\tau) \rangle}{\langle \Psi_v | \Psi(\tau) \rangle} = \frac{\langle \Psi(\frac{\tau}{2}) | \hat{H} | \Psi(\frac{\tau}{2}) \rangle}{\langle \Psi(\frac{\tau}{2}) | \Psi(\frac{\tau}{2}) \rangle},$$

(5)

provides an upper bound which approaches the lowest-energy eigenvalue with quantum numbers $\xi$ in the limit $\tau \to \infty$. The values of $E(\tau)$, calculated from 10,000 configurations for each of the three 6N states and 20,000 configurations for $^4He$ are shown in Fig. [I] along with their statistical error estimates. The $^4He$ $E(\tau)$ decreases from the variational energy $E_v = E(\tau = 0)$ by $\sim 1.2$ MeV in $\sim 0.02 MeV^{-1}$, and is almost independent of $\tau$ thereafter, suggesting that the $\Psi_v$ has $\leq 2\%$ admixture of states with excitation energy $\geq 50$ MeV. The $E(\tau)$ of the 6N states, in contrast, decreases by $\sim 4$ MeV from $E_v$, and does not appear to have reached the $\tau \to \infty$ asymptotic value at $\tau = 0.06 MeV^{-1}$. The statistical error, governed by variance of $\hat{H}\Psi_v(R)/\Psi_v(R)$ is larger in the 6N $E(\tau)$. These indicate that the 6N $\Psi_v$ are not as accurate as the $^4He$ $\Psi_v$, and that they need to be improved for more accurate GFMC calculations.

The average value of $E(\tau)$ in the $\tau$ interval 0.03 to 0.06 MeV$^{-1}$ is listed as $\bar{E}$ in Table I. The $\bar{E}$ of $^3H$, $^4He$, and $^5He$ can be identified with their ground state energies, however, those of the 6N states can only be regarded as upper bounds. It is difficult to extrapolate the 6N $E(\tau)$ to $\tau \to \infty$, particularly due to the large statistical errors; nevertheless we have attempted it in the following way. Let $\Psi_i$ be the eigenstates with quantum numbers $\xi$ and energies $E_i$. The $\Psi_v$ contains admixtures of $\Psi_i$ with amplitude $\beta_i$ in addition to the $\Psi_o$ of the lowest-energy state. Admixtures with the smallest $E_i - E_o$ determine the behavior of $E(\tau)$ at large $\tau$. We approximate the contribution of low-lying states with two delta functions at $E_1$ and $E_2$ with amplitudes $\beta_1$ and $\beta_2$. It is experimentally known that the lowest $T = 0$, $J^\pi = 1^+(3^+)$ resonances in $^6Li$ are $5.65(\sim 13.6)$ MeV above the $1^+(3^+)$ bound states [13]. Accordingly, we assume that $E_1 - E_o = 5.65(13.6)$ MeV for the $1^+(3^+)$ states and also use the value 13.6 for $T = 1$, $J^\pi = 0^+$. Further assuming that $E_2 - E_o = 30$ MeV the calculated values of $E(\tau > 0.01 MeV^{-1})$ are fitted by varying $E_o$, $\beta_1$, and $\beta_2$. Fortunately, the fits are not very sensitive to $E_2 - E_o$, and are shown in Fig. [I]. The resulting value of $E_o$ is listed as
the calculated energy in Table I. The error in the extrapolated $E_o$ is much larger than that in $\bar{E}$ and less reliable.

The expectation values of various terms in the Hamiltonian are also listed in Table I. These are averages over the interval $\tau = 0.03$ to $0.06 MeV^{-1}$, calculated using

$$\langle \hat{O}(\tau) \rangle = 2 \frac{\langle \Psi_v | \hat{O} | \Psi(\tau) \rangle}{\langle \Psi_v | \Psi(\tau) \rangle} - \frac{\langle \Psi_v | \hat{O} | \Psi_v \rangle}{\langle \Psi_v | \Psi_v \rangle},$$

(6)
correct up to order $|\Psi(\tau)\rangle - |\Psi_v\rangle$. The dominant $\langle v_{14} \rangle$ and $\langle K \rangle$ have similar values in $^4He$ and $^5He$; while in the 6N states they are closer to the sum of their values in $^4He$ and $^2H$. The $\langle V_{ijk} \rangle$ are similar in $^4He$, $^5He$, and 6N states. The $\langle v_{LS} \rangle$ contains both $L S$ and $L S(\tau_i \tau_j)$ terms in the NN interaction. They contribute, along with $V_{ijk}$, to the splitting between $\frac{3}{2}^-$ and $\frac{1}{2}^-$ states of $^5He$. However, the calculated splitting of 0.8(3) MeV is much smaller than the observed 1.4 MeV. The magnitudes of $\langle v_{LS} \rangle$ and $\langle V_{ijk} \rangle$ are larger in the 6N 0$^+$ and 3$^+$ states than in the 1$^+$, suggesting that the 1$^+$ has less contribution from the $(p\frac{3}{2})^2$ configuration than the other two. The underbinding of the 6N 0$^+$ and 3$^+$ states by $\sim 1$ MeV is probably related to that of the $^5He \frac{3}{2}^-$ state. In $^5He$, only the expectation value $\langle v_{pp}^{coul} \rangle$ of the Coulomb interaction between protons is calculated. The other terms in $\langle v_{em} \rangle$ for $^5He$ (given in parentheses in Table I) are estimated from results for $^4He$ and $^6He$. The $\langle v_{pp}^{coul} \rangle$ decreases by $\sim 5\%$ from $^4He$ to $^6He$ indicating that the $\alpha$-cluster expands as we go from $A = 4$ to 6.

The last three lines of Table I give rms proton and neutron radii. The calculated values of $R(p)$ compare well with the those extracted from observed charge radii [17]. The experimental $R(p)$ of $^3He$ is 1.77 fm, in reasonable agreement with the calculated $R(n)$ of $^3H$. The Coulomb interaction accounts for most of the isovector $^6Be - ^6He$ difference (Table II). Since this difference is correctly predicted, the $R(p)$ of $^6Be$, assumed to be equal to the $R(n)$ of $^6He$, appears to have a reasonable value.

The contributions of $v_{em}$, $v_{cib}$, $v_{csb}$, and $K_{csb}$, treated as first order perturbations in this work, are responsible for the energy differences within the $T = \frac{1}{2}$ and $T = 1$, $J^\pi = 0^+$ 6N multiplets listed in Table II. The present Hamiltonian explains the isovector energy
differences $^3\text{He} -^3\text{H}$ and $^6\text{Be} -^6\text{He}$ fairly well. The three-body calculations show that the isovector $v_{csb}$ and $K_{csb}$ are necessary to obtain the observed $^3\text{He} -^3\text{H}$ difference, in agreement with earlier results of Faddeev calculations [18]. Unfortunately, the calculated value of the isotensor difference $\frac{1}{2}(^6\text{Be} + ^6\text{He}) - ^6\text{Li}$ is much larger than observed. The observed difference is essentially explained by the electromagnetic interaction alone. This is very puzzling because most of the contribution of the isotensor $v_{cib}$ to this difference should be from the relative $^1S_0$ two-nucleon state in which the difference between $pp$ and $np$ phase shifts seems to be well established [19,20]. The nonperturbative contribution of the Coulomb interaction, particularly in $^6\text{Be}$, neglected here, may reduce the value of this isotensor difference. There could also be some contribution from charge-dependence of the two-pion exchange $V_{ijk}$.

In conclusion, we have demonstrated that the GFMC method can be used to accurately calculate the energies of the many nuclear states with $A \leq 6$ from realistic models of nuclear forces. It appears possible to extend these calculations to several $A = 7$ and 8 states by using larger parallel computers such as the IBM SP2. The calculated energies are in good agreement with experiment. However, some differences, such as the underestimation of the splitting between $\frac{3}{2}^-$ and $\frac{1}{2}^-$ states of $^5\text{He}$ are clearly established. We could attempt to probe relativistic effects [21,22], and the spin-isospin dependence of the short-range part of the $V_{ijk}$ using these differences. A detailed analysis of the GFMC wave function $e^{-\hat{H}\tau}\Psi_{v}$ is in progress to study the structure of the 6N states and improve upon their $\Psi_{v}$.

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FIGURES

FIG. 1. The top to bottom data sets show the $E(\tau)$ for $^{6}\text{He}$, $^{6}\text{Li}(3^{+})$, $^{4}\text{He}$, and $^{6}\text{Li}(1^{+})$ states, along with the fits described in the text. Constants of 2.5, 1.5, and 0.5 MeV have been added to the $E(\tau)$ of $^{6}\text{He}$, $^{6}\text{Li}(3^{+})$, and $^{4}\text{He}$, respectively, for clarity.
TABLE I. Calculated energies and radii in MeV and fm.

| Nucleus (J) | $^2H(1)$ | $^3H(\frac{1}{2})$ | $^4He(0)$ | $^5He(\frac{3}{2})$ | $^5He(\frac{1}{2})$ | $^6He(0)$ | $^6Li(1)$ | $^6Li(3)$ |
|-------------|----------|-----------------|-----------|-----------------|-----------------|-----------|-----------|-----------|
| E(Expt.)    | −2.22    | −8.48           | −28.3     | −27.2           | −25.8           | −29.3     | −32.0     | −29.8     |
| E(Calc.)    | −2.22    | −8.47(2)        | −28.3(1)  | −26.5(2)        | −25.7(2)        | −28.2(8)  | −32.4(9)  | −28.9(6)  |
| $\bar{E}$  | −2.22    | −8.47(2)        | −28.3(1)  | −26.5(2)        | −25.7(2)        | −27.3(4)  | −31.1(4)  | −28.2(3)  |
| $\langle K \rangle$ | 19.9  | 50.(1)          | 118.(1)   | 122.(2)         | 117.(2)         | 146.(4)   | 143.(3)   | 138.(3)   |
| $\langle v_{14} \rangle$ | −22.1 | −58.(1)         | −142.(1)  | −145.(2)        | −140.(2)        | −172.(4)  | −173.(3)  | −165.(3)  |
| $\langle V_{ijk} \rangle$ | 0  | −1.20(3)        | −6.5(3)   | −7.0(4)         | −6.4(4)         | −7.0(7)   | −6.2(6)   | −6.9(5)   |
| $\langle v_{LS} \rangle$ | −0.08 | −0.20(5)        | −0.4(1)   | −1.2(1)         | −0.4(1)         | −2.7(3)   | −1.5(5)   | −3.0(4)   |
| $\langle v_{em} \rangle$ | 0.018 | 0.039(1)        | 0.879(5)  | (0.86)          | (0.86)          | 0.87(1)   | 1.71(2)   | 1.72(2)   |
| $\langle v_{pp}^{coul} \rangle$ | 0. | 0.761(2)        | 0.745(3)  | 0.751(3)        | 0.724(8)        | 1.55(2)   | 1.57(2)   |           |
| R(n)        | 1.967    | 1.72            | 1.42(1)   | 3.02(3)         | 3.57(3)         | 2.62(1)   | 2.41(5)   | 2.46(7)   |
| R(p)        | 1.967    | 1.58            | 1.42(1)   | 1.84(2)         | 1.99(2)         | 1.89(6)   | 2.41(5)   | 2.46(7)   |
| R(p)(Expt.) | 1.953    | 1.61            | 1.47      |                |                |           |           | 2.43      |

TABLE II. Energy differences in MeV within isospin multiplets

|            | $^3He - ^3H$ | $^6Be - ^6He$ | $\frac{1}{2}(^6Be + ^6He) - ^6Li$ |
|------------|-------------|--------------|----------------------------------|
| $\langle v_{em} \rangle$ | 0.669 | 2.33 | 0.33  |
| $\langle K_{csb} \rangle$ | 0.014 | 0.036 | 0   |
| $\langle v_{csb} \rangle$ | 0.066 | 0.116 | 0   |
| $\langle v_{cib} \rangle$ | 0 | 0 | 0.28 |
| $\Delta(Calc.)$ | 0.749(1) | 2.5(1) | 0.6(1) |
| $\Delta(Expt.)$ | 0.764 | 2.35 | 0.34 |
\[6Li\quad 1^+\]
\[6Li\quad 3^+\quad (+1.5\text{ MeV})\]
\[6He\quad 0^+\quad (+2.5\text{ MeV})\]
\[4He\quad 0^+\quad (+0.5\text{ MeV})\]

**Graph:**
- **Y-axis:** \(E(\tau)\) (MeV)
- **X-axis:** \(\tau\) (1/MeV)

The graph shows the energy \(E(\tau)\) in MeV as a function of \(\tau\) in 1/MeV, with error bars indicating uncertainty. Different symbols represent different isotopes:
- **Black circle:** \(6Li\quad 1^+\)
- **Black square:** \(6Li\quad 3^+\quad (+1.5\text{ MeV})\)
- **Black diamond:** \(6He\quad 0^+\quad (+2.5\text{ MeV})\)
- **Black square with diamond:** \(4He\quad 0^+\quad (+0.5\text{ MeV})\)