# VARIATIONAL MONTE CARLO CALCULATIONS OF FEW-BODY NUCLEI

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## Abstract

The variational Monte Carlo method is described. Results for the binding energies, density distributions, momentum distributions, and static longitudinal structure functions of the $^3$H, $^3$He, and $^4$He ground states, and for the eneriges of the low-lying scattering states in $^4$He are presented.

The variational Monte Carlo (VMC) method has been used for a wide variety of studies in both few- and many-body systems. These include calculations of the ground state binding energy and density of infinite liquid atomic $^3$He and $^4$He [1-3] and of liquid drops containing up to 240 atoms of $^3$He or $^4$He [4,5]. This note will review the application of VMC methods to nuclear few-body systems [6-13]. New results using the 34-channel Faddeev wave function of the Los Alamos-Iowa group [14,15] confirm the binding energy and density distributions reported by them, and present the first momentum distribution and longitudinal structure function calculations with these wave functions.

In the VMC method a variational wave function $\psi_V(\alpha)$ is constructed (with parameters denoted by $\alpha$) and a Rayleigh-Ritz upper bound to the ground-state energy,

$$E_V(\alpha) = \frac{\langle \psi_V(\alpha) | H | \psi_V(\alpha) \rangle}{\langle \psi_V(\alpha) | \psi_V(\alpha) \rangle} \geq E_0 \qquad (1)$$

is evaluated. The Metropolis Monte Carlo algorithm [16] is used for the 3A-dimensional integration. The parameters $\alpha$ are varied until the lowest upper bound is found; the resulting $E_V$ is taken as the energy of the system, and other properties are computed using $\psi_V$.

The VMC method has several advantages. In particular it has wide applicability to problems in both nuclear and condensed matter physics. The general structure for good candidate $\Psi_V$ is well established both from the VMC studies of atomic helium systems and from variational hypernetted chain (HNC) studies of nuclear matter [7,10,17,18]. The Monte Carlo integration procedure can provide arbitrary accuracy (althought at the cost of a quadratic increase in computer time) and no partial-wave expansion for the Hamiltonian, or any other operator, is required.

The chief disadvantage is that the wave function is variational. Better wave functions can generally be found when more exact methods can be brought to bear, e.g., the recent Faddeev calculations for $^3$H [14,15,19,20] or the Green's function Monte Carlo (GFMC) calculations of atomic helium drops [4]. Further, while variational methods are economical in computer usage for a single evaluation of the energy, a search in the parameter space $\alpha$ must be performed, requiring many energy evaluations to determine the best $\Psi_V$. This determination is made more difficult by the statistical error of the Monte Carlo integration procedure.

In nuclear systems we wish to take the expectation value of a many-body Hamiltonian of the form

$$H = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk} . \qquad (2)$$

The variational wave function for $^3$H and $^4$He is written as [6]

$$\Psi_V = \{ \mathcal{S} \prod_{i<j} F_{ij} \} \Phi , \qquad (3)$$

$$F_{ij} = f_c(r_{ij}) [1 + \sum_{k\neq i,j} f_3(r_{ij}, r_{ik}, r_{jk}) \{u_\sigma(r_{ij})\sigma_i\cdot\sigma_j + u_{t\tau}(r_{ij})S_{ij}\tau_i\cdot\tau_j\} ]. \qquad (4)$$

Here $\mathcal{S}$ is a symmetrizer, $f_c$ provides both short-range correlation and long-range confinement, $f_3$ is a three-body correlation that acts only on the state-dependent correlations $u_\sigma$ and $u_{t\tau}$, and $\Phi$ is an antisymmetrized spin-isospin state. The $f_c$, $u_\sigma$, and $u_{t\tau}$ are obtained from the solution of coupled Euler-Lagrange equations which minimize the two-body cluster energy subject to boundary conditions set to constrain their asymptotic long-range behavior in an appropriate manner for pd and ppn breakup in $^3$He and for pt and dd breakup in $^4$He [11]. In our calcualtions $\Psi_V$ is stored as a vector with $(2^A\, A!/(A-Z)!Z!)$ components, each of which specifies the

Alternatively a Faddeev wave function, $\psi_F$, or any other suitable wave function can be used in the Monte Carlo integrations [9]. In fact, analysis of the 5-channel $\psi_F$ led to a significant improvement in the long-range boundary conditions used for the $\psi_V$ of eq.(3). We are now studying the 34-channel $\psi_F$ for possible further improvements in the variational ansatz that can be applied to $^4$He and larger nuclei.

The Metropolis Monte Carlo algorithm [16] provides a way for drawing points $\{\mathbf{R}_i\}$ in 3A-dimensional space from a normalized probability distribution $P(\mathbf{R}) = |\psi(\mathbf{R})|^2 / \int |\psi(\mathbf{R})|^2 d\mathbf{R}$. The central limit theorem then implies that for any quantity $f(\mathbf{R})$,

$$\lim_{N\to\infty} \frac{1}{N} \sum_i f(\mathbf{R}_i) = \frac{\int |\psi(\mathbf{R})|^2 f(\mathbf{R})\, d\mathbf{R}}{\int |\psi(\mathbf{R})|^2 d\mathbf{R}} , \tag{5}$$

and in particular,

$$E_V = \lim_{N\to\infty} \frac{1}{N} \sum_i \psi^{-1}(\mathbf{R}_i)\, H\, \psi(\mathbf{R}_i) . \tag{6}$$

The binding energy results in $^3$H for several Hamiltonians and wave functions are shown in table 1. The $v_{ij}$ used is the Argonne $v_{14}$ (AV14) model [21] and $V_{ijk}$ is either the Urbana model VII (U7) model [11] or Tucson-Melbourne (TM) model [22]. Three different $\psi_F$ have been used, which were obtained by solving for AV14, AV14+U7, and AV14+TM Hamiltonians, respectively. These expectation values all agree with the values reported by the Los Alamos-Iowa group [14,15]. Also shown are the results obtained by using $\psi_V$ of the form of eq.(3) for both $^3$H and $^4$He. These results are from larger Monte Carlo samplings than (but are consistent with) previously reported values [11].

Table 1. Binding energies in MeV for $^3$H and $^4$He for different H and $\psi$. Numbers in parentheses are one-standard-deviation Monte Carlo sampling errors.

| | | AV14 | AV14+U7 | AV14+TM |
|---|---|---|---|---|
| $^3$H | $\psi_F$ (AV14) | 7.68 (2) | 8.71 (4) | 8.41 (4) |
| | $\psi_F$ (AV14+U7) | 7.27 (4) | 9.04 (3) | 8.56 (3) |
| | $\psi_F$ (AV14+TM) | 6.50 (4) | 8.24 (4) | 9.332 (15) |
| | $\psi_V$ (AV14+U7) | 7.05 (4) | 8.28 (4) | 7.35 (6) |
| $^4$He | $\psi_V$ (AV14+U7) | 21.5 (3) | 27.4 (4) | 23.9 (4) |

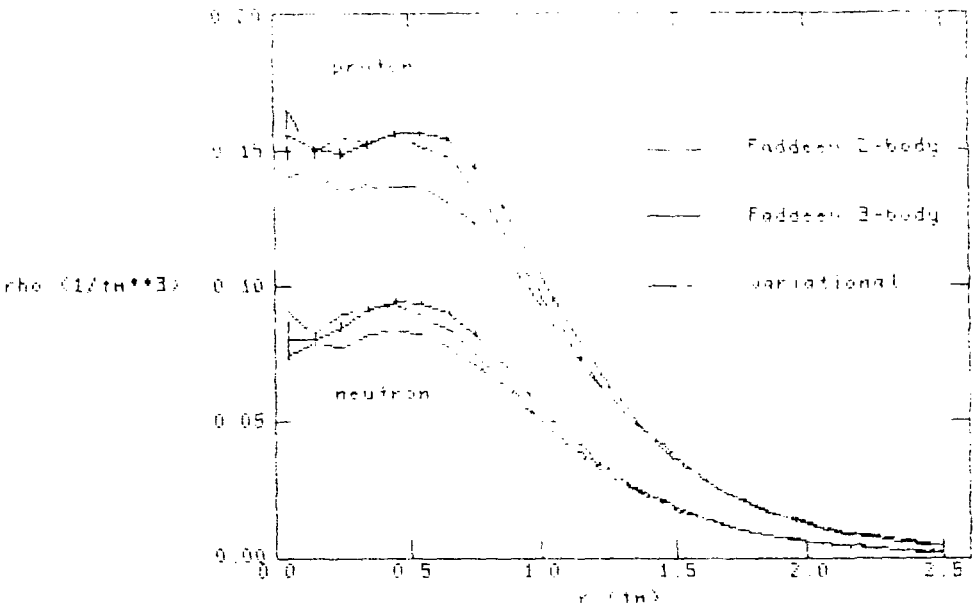


Figure 1. Density distributions in $^3$He for several $\Psi$.

The current $\Psi_V$ gives 0.7 to 0.8 MeV less binding in $^3$H for AV14+U7 than the 34-channel $\Psi_F$. If this deficiency of the variational ansatz scales with the total potential energy, then the true $^4$He binding energy for AV14+U7 might be $\approx$ 29.2 MeV; if it scales as $\langle V_{ijk} \rangle$ the binding energy might be $\approx$ 30.5 MeV.

The proton and neutron density distributions for several of these wave functions are shown in fig. 1. The density for AV14+U7 shows a small central depression, in agreement with the results reported by the Los Alamos-Iowa group.

Nucleon momentum distributions can be evaluated by sampling the quantity

$$N_{tz}(k) = \int d\mathbf{r}_1' \, \Psi_V^{-1}(\mathbf{R}) \exp[i\mathbf{k}\cdot(\mathbf{r}_1'-\mathbf{r}_1)] \, P_{tz}(1) \, \Psi_V(\mathbf{R}') \qquad (7)$$

where $\mathbf{R} = (\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$, $\mathbf{R}' = (\mathbf{r}_1',\mathbf{r}_2,\mathbf{r}_3)$, and $P_{tz}$ is an isospin projection operator. The proton momentum distributions in $^3$He calculated for several wave functions are shown in fig. 2, along with (e,e'p) data analyzed in PWIA [23]. The $N_p(k=0)$ intercept scales as $E^{-3}$ and $\Psi_V$ comes closest to experiment because its binding energy is closer than any of the $\Psi_F$ (even though it is not the best $\Psi_V$ for H). As k increases all the wave

functions give an $N_p(k)$ increasingly above the data. Since these high-k components arise when the nucleons are close together, final state interactions may be expected to play an important role and the PWIA analysis will not be adequate. Calculations in the VMC framework are currently under way to study the final state interactions [24].

Two-body breakup amplitudes can also be calculated giving $N_{dp}(k)$ in $^3$He and $N_{tp}(k)$ and $N_{dd}(k)$ in $^4$He. The $N_{dp}(k)$ exhibit the same behavior as $N_p(k)$, with the k=0 value well predicted, but an increasing disparity with increasing k compared to the PWIA analysis of available (e,e'p) data [10]. The $D_2$ values, which are related to the asymptotic ratio of D-state to S-state wave functions in the d+p and d+d amplitudes, are also computed with $\psi_V$ and give -0.24 and -0.16, respectivley, for AV14+U7.

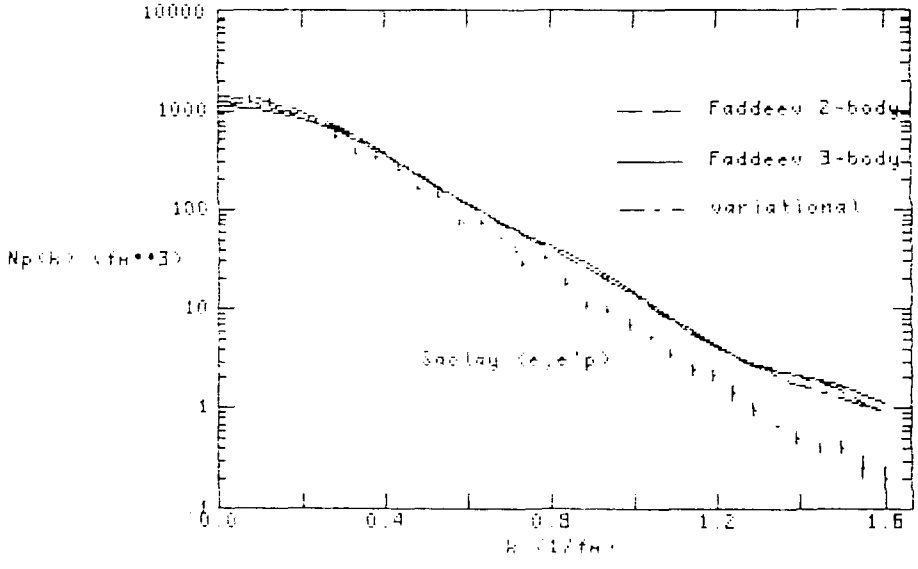


Figure 2. Proton momentum distributions in $^3$He for several $\psi$.

Other quantities of interest are the dynamic and static longitudinal structure functions $S_L(k,\omega)$ and $S_L(k)$,

$$S_L(k,\omega) = {}^1/_2 \sum_f \langle 0|\rho^\dagger_{L,k}|I\rangle \langle I|\rho_{L,k}|0\rangle\, \delta(\omega-\omega_I), \qquad (8)$$

$$\rho_{L,k} = \sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i)\, {}^1/_2\{ (1+\tau_3(i)) - \mu_n\, [k^2/4(k^2+m^2)]\, (1-\tau_3(i)) \}. \qquad (9)$$

$$S_L(k) = \int_{0^+}^{\infty} S_L(k,\omega)\, d\omega \qquad (10)$$

In eq.(8) the sum is over all states $|I\rangle$, $|0\rangle$ is the ground state, and $\omega_I$ is the energy of state I with respect to the ground state. The sum in eq.(9) is over all particles, $^1/_2\,(1\pm\tau_3(i))$ are proton and neutron projection operators, and the $\mu_n$ term comes from electron-neutron scattering. The lower limit of the integral in eq.(10) is taken for convenience as $0^+$ to eliminate the elastic contribution. $S_L(k)$ can be evaluated in the light nuclei by using closure and subtracting the elastic part explicitly:

$$S_L(k) = {}^1/_Z\,[\,\langle 0|\rho^{\dagger}_{L,k}\,\rho_{L,k}|0\rangle - |\langle 0_R|\rho_{L,k}|0\rangle|^2\,]\,. \qquad (11)$$

Here the recoiling ground state $|0_R\rangle = \exp(^1/_A\Sigma\,\mathbf{k}\cdot\mathbf{r}_i)\,|0\rangle$, and the expectation values in eq.(11) are easily evaluated by Monte Carlo integration. The results of such calculations using $\psi_V$ for $^3$H, $^3$He, and $^4$He are shown in fig. 3, along with experimental data on $^3$He [25]. The calculations agree with experiment very well; substitution of $\psi_F$ does not significantly alter the reuslts. The calculation of $S_L(k,\omega)$ is more involved, but is currently underway [24].

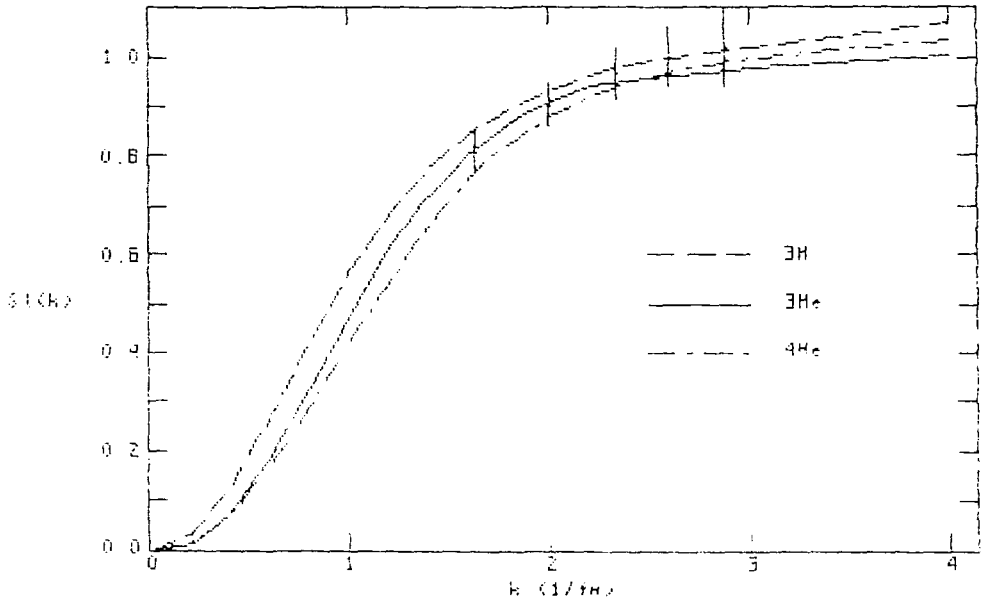


Figure 3. Static longitudinal structure function $S_L(k)$.

The VMC method has also been used to study the excited resonance states in $^4$He [8]. This is done with a modified R-matrix method which converts the scattering problem into a bound-state problem with special boundary conditions. The variational wave function for the excited states is taken as:

$$\Psi_V(J^\pi,T,n) = \left( \mathcal{S} \prod_{i<j} F_{ij} \right) \varphi(J^\pi,T,n) , \tag{12}$$

$$\varphi(J^\pi,T,n) = \left[ \sum_i \xi_{nl}(\mathbf{R}_i)\, O_i(J^\pi,T) \right] \varphi . \tag{13}$$

Here the correlation operator of eq.(4) is now applied to an uncorrelated excited state $\varphi(J^\pi,T,n)$, which is constructed from a sum over single particles i of a radial wave function $\xi_{nl}(\mathbf{R}_i \equiv A[\mathbf{r}_i - \mathbf{R}_{c.m.}]/[A-1])$ with nodal and angular quantum numbers n and l, and an operator $O_i(J^\pi,T)$ of angular momentum J, parity $\pi$, and isospin T. For $^4$He the lowest excited states are $(J^\pi,T) = (0^+,0)$, $(0^-,0)$, and $(2^-,0)$; the corresponding (n,l) values are (1,0), (0,1), and (0,1), and the $O_i$ are 1, $\boldsymbol{\sigma}_i \cdot \mathbf{R}_i$, and $3\boldsymbol{\sigma}_{3i} \cdot \mathbf{R}_{3i} - \boldsymbol{\sigma}_i \cdot \mathbf{R}_i$, respectively. The radial dependence of $\xi_{nl}$ is controlled by a few variational parameters, while $F_{ij}$ is taken from the ground state calculation.

The excited state energy $E(J^\pi,T,n)$ is the expectation value of eq.(1) with $\Psi_V(J^\pi,T,n)$ substituted for $\Psi_V$. If we ignore the Coulomb force, the $(0^+,0)$ state is weakly bound and can be treated as a regular variational problem. Because the $(J^\pi,T)$ quantum numbers are the same as the ground state, $E(0^+,0,1)$ is minimized subject to the orthogonality conditon $\langle \Psi_V(0^+,0,1) | \Psi_V \rangle = 0$. For the negative parity states we calculate the phase shift $\delta_l$,

$$\tan(\delta_l) = j_l(kR_n)/n_l(kR_n) , \tag{14}$$

$$k = \left( 2\mu E_{rel}/\hbar^2 \right)^{1/2} , \tag{15}$$

$$E_{rel} = E(J^\pi,T,n) - E(^3H) . \tag{16}$$

Here $E_{rel}$ is the relative energy of a proton scattering off $^3$H. It is obtained by picking a nodal boundary $R_n$ where $\xi_{nl}(R_n) = 0$, and minimizing $E(J^\pi,T,n)$ inside this boundary. The calculation is performed for several values of $R_n$, thus mapping out $\delta(E)$. Both the $0^-$ and $2^-$ states show resonant behavior, and the energy at which $\partial\delta(E)/\partial E$ is a maximum is identified as the energy of the resonance.

In the calculation for $^4$He, the states come out in the correct order, with the $0^+$ state at -8.6 ± 0.4 MeV, and the $0^-$ and $2^-$ states at -6.5 ± 0.5 MeV and -4.0 ± 0.5 MeV, which may be compared to Coulomb corrected experimental values of -8.5, -7.4, and -6.4, respectively. The $V_{ijk}$ contributes significantly to the excitation by lowering the ground state energy much more than the resonance states, as one would expect. More recently, this method has been applied by the Courant group to the five-body problem of $\alpha$-neutron scattering [13]. They calculate both the $J=^1/_2$ and $^3/_2$ scattering states using a semirealistic $v_{ij}$ and a $V_{ijk}$ and obtain most of the observed spin-orbit splitting without recourse to relativistic effects.

Future work with the VMC method will involve 1) improving the ansatz for constructing $\Psi_V$, 2) extending the calculations to more properties of interest, 3) extending the calculations to larger nuclei, and 4) further refining the nuclear many-body Hamiltonian. The improvements in $\Psi_V$ include the introduction of $\mathbf{L}\cdot\mathbf{S}$ correlations and better three-body correlations. The 34-channel $\Psi_F$ sets a goal for performance in $^3$H, and any improvements we can make there should carry over to the larger systems. The study of final state interactions in (e,e'p) scattering and of $S_L(k,\omega)$ are examples of additional properties beyond the ground-state binding energy that can be calculated [24]. Meson-exchange currents are another area that should be investigated.

The extension to larger systems has already begun with a first calculation of $^{16}$O by the Courant group [10]. Using the semirealistic Reid $v_6$ interaction (containing tensor, but no spin-orbit forces) they obtain a binding energy per particle of -6 ± 1 MeV. The calculation is computationally very time consuming, and further improvement in the algorithm is necessary, as well as the use of more realisitic interactions. Nevertheless, with the continuing rapid increase in computer power, such microscopic calculations may become commonplace in a few years. Realistic studies of smaller systems like $^6$Li and $^8$He are probably feasible now.

The long term goal of all these studies is the improvement of our understanding of the nuclear many-body Hamiltonian. The VMC method will continue to be a quantitatively valuable tool in the study of possible interactions, e.g. in the study of alternative $V_{ijk}$ models [12]. Future work may include the study of $v_{ij}$ models with explicit $\Delta$ components, as

a possible alternative to $V_{ijk}$ [19,21] or the study of semirelativistic H where the consequences of using $\sqrt{p^2+m^2}$ for the kinetic energy may be explored.

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