Benchmark test calculation of a four-nucleon bound state

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In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8′ *NN* interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

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I. INTRODUCTION

Recent advances in computational facilities, together with the development of new methods and refinements upon older ones, allow very precise calculations for few-body systems. These advances are especially remarkable in nuclear physics considering the complexity of the nuclear interaction. The three-nucleon ($3N$) bound-state [1–3] and scattering-state [4–6] problems are rigorously solved using realistic nuclear potentials [7–9]. These calculational schemes are mostly based on a partial wave decomposition. Stochastic and Monte Carlo methods for bound states, however, are performed directly using position vectors in configuration space. Also in momentum space the first steps have been taken to avoid partial wave decompositions in both two-nucleon (NN) [10] and $3N$ [11,12] systems. Benchmark calculations based on different algorithms for the $3N$ continuum both below [13,14] and above [15] the deuteron threshold already exist.

The complicated calculation of few-body continuum states can be avoided in the evaluation of reaction cross sections, even in the presence of realistic forces [16]. In fact the transition strength can be calculated in an alternative way, where only bound state techniques are needed [17].

There are a few analytical solutions of $3N$ bound states [18] for square-well potentials, against which numerical solutions have been checked, but they are far from possessing the complexity of realistic nuclear forces. In the four-body system we are only aware of benchmark calculations for four bosons [3].

Benchmark calculations are extremely useful to test methods as well as calculational schemes. They are also often of interest for a general readership, since they may help to solve analogous problems in other fields. We think that this is particularly the case for the quite complex four-fermion system. Here we would like to address the four-nucleon ($4N$) bound-state problem using the AV8′ NN potential [19] which is a simplified, reprojected version of the fully realistic Argonne AV18 model [8], but still has most of its complexity, e.g., the tensor force is built in.

In Sec. II the different methods are briefly introduced and the results are presented in Sec. III together with a brief summary.

II. METHODS

In order to solve the bound four-nucleon system we employ the Faddeev-Yakubovsky equations (FY) [20–23], the coupled-rearrangement-channel Gaussian-basis variational method (CRCGV) [24–31], the stochastic variational method (SVM) with correlated Gaussians [32–35], the hyperspherical harmonic variational method (HH) [36–41], the Green's function Monte Carlo (GFMC) [42,43,19,44] method, the no-core shell model (NCSM) [45–47], and the effective interaction hyperspherical harmonic method (EIHH) [48]. The various procedures are briefly described below.

A. Faddeev-Yakubovsky equations

The $4N$ Faddeev-Yakubovsky equations in momentum space are [21–23]

$$\psi_1 = G_0 t_{12} P[(1-P_{34})\psi_1 + \psi_2], \tag{1}$$

$$\psi_2 = G_0 t_{12} \tilde{P}[(1-P_{34})\psi_1 + \psi_2], \tag{2}$$

where ψ_1 and ψ_2 are Yakubovsky components and t_{12} is the two nucleon transition matrix determined by a two nucleon Lippmann-Schwinger equation. P, P_{34}, and $\tilde{P}$ are permutation operators: $P=P_{12}P_{23}+P_{13}P_{23}$, $\tilde{P}=P_{13}P_{24}$, where the P_{ij} are transpositions of particles i and j. The fully antisymmetrized wave function Ψ is

$$\Psi = [1-(1+P)P_{34}](1+P)\psi_1 + (1+P)(1+\tilde{P})\psi_2. \tag{3}$$

The Yakubovsky equations are decomposed into partial waves. We truncate the partial waves at a two-body total angular momentum $j \leqslant 6$, all other orbital angular momenta at $l_i \leqslant 8$, and the sum of all angular momenta at $\Sigma_i l_i \leqslant 12$. In this truncation we keep 1572 angular momentum and isospin combinations (often called channels). This is sufficient to guarantee convergence of our results as given in Sec. III. The diagonalization is performed by a modified Lanczos method [49]. Recent results for realistic NN potentials, and including three-nucleon forces, are given in [22].

B. Coupled-rearrangement-channel Gaussian-basis variational method

The coupled-rearrangement-channel Gaussian basis variational method was proposed by Kamimura [24] to solve the Coulombic three-body problem of the muonic molecular ion $(dt\mu)^+$, within an accuracy of seven significant figures for the energy of the very loosely bound $J=v=1$ state; this accuracy was required for the comparison with experimental data on the muon catalyzed fusion cycle. Use of basis functions that spanned all the three rearrangement Jacobian coordinates was essential to the high-precision calculation. The method was also applied to three-nucleon bound states [25,26] and was found to accomplish a much more rapid convergence in the binding energy with respect to the number of the three-body angular momentum channels (see Fig. 5 of [26]).

The method was also successfully used to make another high-precision Coulomb three-body calculation of the antiprotonic helium atom $(\bar{p}+\mathrm{He}^{++}+e^-)$ in highly excited metastable states with $J \approx 35$ [27]. The calculation agreed with the high-resolution laser spectroscopic data within seven significant figures so that the mass of antiproton was derived to two orders of magnitude better precision than published values. The method has been useful in four-body calculations of the structure of light hypernuclei with realistic YN and NN interactions [28–30].

The total four-body wave function is described as the sum of amplitudes of the rearrangement-Jacobian-coordinate channels with the LS coupling scheme

$$\Psi_{JM} = \sum_\alpha C_\alpha^{(K)} \Phi_\alpha^{(K)} + \sum_\alpha C_\alpha^{(H)} \Phi_\alpha^{(H)}, \tag{4}$$

where antisymmetrized basis functions are described with quantum numbers $\alpha \equiv \{nl, NL, \Lambda, \nu\lambda, I, ss'S, t\}$ by

$$\Phi_\alpha^{(K)} = \mathcal{A}\{([[[\phi_{nl}(\mathbf{r})\psi_{NL}(\mathbf{R})]_\Lambda \varphi_{\nu\lambda}(\boldsymbol{\rho})]_I \times [[\chi_s(12)\chi_{1/2}(3)]_{s'}\chi_{1/2}(4)]_S)_{JM} \times [[\eta_t(12)\eta_{1/2}(3)]_{1/2}\eta_{1/2}(4)]_0\}, \quad (5)$$

$$\Phi_\alpha^{(H)} = \mathcal{A}\{([[[\phi_{nl}(\mathbf{r}')\psi_{NL}(\mathbf{R}')]_\Lambda \varphi_{\nu\lambda}(\boldsymbol{\rho}')]_I \times [\chi_s(12)\chi_{s'}(34)]_S)_{JM}[\eta_t(12)\eta_t(34)]_0\}. \quad (6)$$

We employ *K*-type coordinates $\mathbf{r}=\mathbf{x}_1-\mathbf{x}_2$, $\mathbf{R}=(\mathbf{x}_1+\mathbf{x}_2)/2-\mathbf{x}_3$, $\boldsymbol{\rho}=(\mathbf{x}_1+\mathbf{x}_2+\mathbf{x}_3)/3-\mathbf{x}_4$ and *H*-type ones $\mathbf{r}'=\mathbf{x}_1-\mathbf{x}_2$, $\mathbf{R}'=\mathbf{x}_3-\mathbf{x}_4$, $\boldsymbol{\rho}'=(\mathbf{x}_1+\mathbf{x}_2)/2-(\mathbf{x}_3+\mathbf{x}_4)/2$. $\mathcal{A}$ is the four-nucleon antisymmetrizer and χ's and η's are the spin and isospin functions, respectively. The functional form of $\phi_{nl}(\mathbf{r})$ is taken as

$$\phi_{nlm}(\mathbf{r}) = r^l e^{-(r/r_n)^2} Y_{lm}(\hat{\mathbf{r}}), \quad (7)$$

where the Gaussian range parameters are chosen to lie in a geometrical progression ($r_n = r_1 a^{n-1}; n = 1 \sim n_{\max}$), and similarly for the other functions ψ and φ. This manner of choosing the range parameters is very suitable for describing both the short-range correlations and the long-range asymptotic behavior precisely [25,31].

Eigenenergies and wave-function coefficients *C*'s are determined by solving the Schrödinger equation with the Rayleigh-Ritz variational principle. It is to be emphasized that truncation is not made for the partial waves of the *NN* interaction, in contrast to the Faddeev-Yakubovsky method, but is done only for the angular momenta of basis functions, as in most variational methods. This makes it possible to accomplish a very quick convergence; the result in Sec. III uses $l, L, \lambda \leqslant 2$ (this is the same as in the case of the three nucleon bound states, mentioned above). For instance, this amounts to 100 channels for the calculation in Sec. III.

C. Stochastic variational method

The correlated Gaussian trial function is written in the following form [32–34]:

$$\Psi = \sum_{i=1}^{\mathcal{K}} c_i \mathcal{A}\left\{ [\theta_{Li}(\hat{\mathbf{x}})\xi_{Si}]_{JM}\xi_{TM_T i}\exp\left(-\frac{1}{2}\mathbf{x}A_i\mathbf{x}\right)\right\}, \quad (8)$$

where $\mathcal{A}$ is the antisymmetrizer, $\mathbf{x}$ stands for a set of $A-1$ intrinsic coordinates $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_{A-1})$ and ξ_{SMi} ($\xi_{TM_T i}$) is the spin (isospin) function of the *A*-particle system. These functions are constructed by successively coupling the spin (isospin) of the nucleons

$$\xi_{SMi} = ([[\chi_{1/2}(1)\chi_{1/2}(2)]_{s_{12}}\chi_{1/2}(3)]_{s_{123}} \ldots)_{SMi} \quad (9)$$

(similarly for the isospin part). The nonspherical (orbital) part of the trial function is represented by a successively coupled product of spherical harmonics

$$\theta_{LMi}(\hat{\mathbf{x}}) = [([Y_{l_1}(\hat{\mathbf{x}}_1)Y_{l_2}(\hat{\mathbf{x}}_2)]_{l_{12}}Y_{l_3}(\hat{\mathbf{x}}_3))_{l_{123}} \ldots]_{LMi}. \quad (10)$$

The index *i* in the above equation stands for a label to distinguish the different possible intermediate coupling schemes as well as the different possible total spin and total orbital angular momentum.

The expansion over the partial waves has to be truncated, but the correlations included in the Gaussian part, $\exp(-\frac{1}{2}\mathbf{x}A_i\mathbf{x})$, make the trial function flexible enough, so these truncations are not expected to seriously affect the accuracy. In the present calculation we included all partial waves up to

$$\sum_{i=1}^{A-1} l_i \leqslant 4. \quad (11)$$

The trial function contains $A(A-1)/2$ nonlinear variational parameters. The total spin, total orbital angular momentum and intermediate coupling quantum numbers are also variational parameters in the sense that one has to include all possibilities which improve the energy. We have a large number of parameters to be optimized and it is not at all clear how to select the optimal quantum numbers.

This variational basis is nonorthogonal, none of the components is indispensable, and one can replace a component by a linear combination of others. This gives us an excellent opportunity to use a stochastic optimization procedure. To optimize the variational basis we used the ''stochastic variational method'' [32–35]. In the SVM one searches for the best wave function by a random trial and error procedure. Random trial functions are generated and their energies are compared. Randomness in this case means that the quantum numbers and the nonlinear parameters are random numbers. Trial functions giving the lowest energy are selected as basis states. Details and various applications of the approach can be found in [32–35].

The number of basis states used in the calculations is about 150 for the triton and 300 for the alpha particle. Very small bases already give quite acceptable results, for the alpha particle, for example, 50 basis states give the binding energy within 1 MeV. The SVM results seem to be convergent in the model space defined with 300 basis states and the partial-wave truncation with $\Sigma_{i=1}^{A-1} l_i \leqslant 4$. We have tried to increase the accuracy by adding 700 more states and by including the partial waves up to $\Sigma_{i=1}^{A-1} l_i \leqslant 6$ but the results are practically unchanged. The 1000 bases give only 2 keV gain in energy. The enlargement of the basis improves the expectation values, especially that of the kinetic energy operator, but this change is canceled by a similar change in the central potential. We think that the upper bound provided by the SVM calculation is very close to the exact energy. The accuracy achieved with few basis dimension is due to the use of the correlated Gaussian basis and the efficient optimization procedure.

D. Hyperspherical harmonic variational method

The hyperspherical harmonic (HH) functions constitute a general basis for expanding the wave functions of an *A*-body system [36–38]. Very precise results can be obtained for the

three-nucleon bound state [39]. In the HH variational method, the wave function is written as

$$\Psi = \sum_{\mu} u_{\mu}(\rho)\Phi_{\mu}^{(K)}, \tag{12}$$

where ρ is the hyper-radius. The quantities $\Phi_{\mu}^{(K)}$ are fully antisymmetrized HH-spin-isospin functions of quantum numbers $\mu \equiv \{n,m,l_1,l_2,l_3,l_{12},L,s,s',S,t,t',T\}$ constructed using the K-type Jacobi coordinates $\mathbf{x}_{1,2,3}$. Explicitly,

$$\begin{aligned}\Phi_{\mu}^{(K)} = \mathcal{A}&((\sin\beta)^{2m}P_n^{\nu,l_3+1/2}(\cos 2\beta)P_m^{l_1+1/2,l_2+1/2}(\cos 2\gamma)\\ &\times[[\eta_t(12)\eta(3)]_{t'}\eta(4)]_{TT_z}(x_1)^{l_1}(x_2)^{l_2}(x_3)^{l_3}\\ &\times\{[[Y_{l_1}(\hat{x}_1)Y_{l_2}(\hat{x}_2)]_{l_{12}}Y_{l_3}(\hat{x}_3)]_L\\ &\times[[\chi_s(12)\chi(3)]_{s'}\chi(4)]_S\}_{JJ_z}),\end{aligned} \tag{13}$$

where $\cos\beta = x_3/\rho$, $\cos\gamma = x_2/(\rho\sin\beta)$ and χ and η denote spin and isospin functions, respectively. Moreover, $\nu = l_1 + l_2 + 2m + 2$ and $P_n^{a,b}$ are Jacobi polynomials (the integers n and m range from zero to infinity). The coefficients $u_{\mu}(\rho)$ depend on the hyper-radius $\rho = \sqrt{(x_1)^2+(x_2)^2+(x_3)^2}$ and can be determined by solving a set of second-order differential equations derived from the Rayleigh-Ritz variational principle. For $A=4$ the necessary matrix elements of the potential have been calculated by exploiting the techniques discussed in Ref. [40].

The main difficulty in applying the HH technique to nuclear systems is the very slow convergence of the expansion due to the strong repulsion between the particles at short distances. In the $A=4$ case, it has been found convenient to separate the HH states in different classes and to study the convergence by including the states of one class at time [41]. The adopted criterion has been to first include the HH functions describing two-body correlations and, successively, those incorporating three- and four-body correlations. Moreover, the HH functions having the lowest orbital angular momentum quantum numbers l_i $(i=1,2,3)$ have been included first.

E. Green's function Monte Carlo method

Green's function Monte Carlo methods use stochastic sampling to evaluate path integrals of the form

$$\Psi_0 = \lim_{\tau\to\infty}\Psi(\tau), \tag{14}$$

$$\Psi(\tau) = e^{-(H-E_0)\tau}\Psi_T, \tag{15}$$

$$= [e^{-(H-E_0)\triangle\tau}]^n\Psi_T, \tag{16}$$

where Ψ_T is an approximate trial function obtained in a variational or in an approximate constrained-path GFMC calculation and we have introduced a small time step, $\tau = n\triangle\tau$. An approximate expression for the propagator,

$$G(\mathbf{R},\mathbf{R}') = \langle \mathbf{R}|e^{-(H-E_0)\triangle\tau}|\mathbf{R}'\rangle, \tag{17}$$

with error proportionate to at least the second power of $\Delta\tau$ is used. In the present work we use a symmetrized product of exact two-body propagators, which has error proportionate to $(\Delta\tau)^3$ [19,44].

Green's function Monte Carlo calculations for light nuclei with spin-isospin dependent interactions sample the particle coordinates while explicitly summing over the spin-isospin degrees of freedom [42]. The first alpha particle calculations including $L\cdot S$ terms employed the Reid V8 interaction [43]. The chief advantage of these methods is that they can be extended to larger nuclei. More computationally efficient versions of the algorithm have been introduced and calculations extended up to $A=8$ [19,44].

Convergence of the ground-state energy is governed by the spectra of the Hamiltonian. Calculations reported here were performed to $\tau = 0.12\ \mathrm{MeV}^{-1}$. Since the first excited state of ^{4}He is above 20 MeV, any errors in Ψ_T are damped out by at least $\exp(-2.4)$, an order of magnitude. In fact our studies show that the errors in Ψ_T correspond to much higher excitation energies and $\langle H\rangle$ converges by $\tau \sim 0.05\ \mathrm{MeV}^{-1}$.

The GFMC method allows us to compute mixed expectation values of the form $\langle\Psi(\tau)|\mathcal{O}|\Psi_T\rangle$. For H, this gives the exact ground state energy if τ is large enough. Expectation values of other quantities, such as pieces of the Hamiltonian, are often obtained through a linear extrapolation in the error of the trial wave function:

$$\langle\Psi(\tau)|\mathcal{O}|\Psi(\tau)\rangle \approx 2\langle\Psi(\tau)|\mathcal{O}|\Psi_T\rangle - \langle\Psi_T|\mathcal{O}|\Psi_T\rangle, \tag{18}$$

though it is possible to go beyond this approximation.

F. No-core shell model method

The NCSM is an approach applicable to both few-nucleon systems as well as to light nuclei [45]. The calculations are performed in a finite model space in the harmonic-oscillator (HO) basis. The model space (P) is spanned by states with the total number of HO quanta $N \leqslant N_{\max}$. The Hamiltonian,

$$H = T + V, \tag{19}$$

is modified by a HO center-of-mass potential. Thus, we work with

$$\begin{aligned}H_A^{\Omega} = &\sum_{i=1}^{A}\left[\frac{p_i^2}{2m} + \frac{1}{2}m\Omega^2 r_i^2\right]\\ &+ \sum_{i<j=1}^{A}\left[V(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2\right].\end{aligned} \tag{20}$$

As the *NN* potential depends on the relative coordinates, the added HO term has no influence on the internal motion in the full space. The effective Hamiltonian, appropriate to the finite P space, is derived by the Hermitian version of the Lee-Suzuki method [46]. In general, the effective Hamiltonian is an A-body operator. We make an approximation by using just a two(three)-body effective interaction, which is obtained by applying the Lee-Suzuki approach to the two(three)-nucleon system using H_A^{Ω} with the sums restricted to two(three) nucleons, but with the A in the interaction term kept fixed to,

e.g., $A=4$ for ^{4}He. Consequently, we deal with a two(three)-nucleon system bound in a HO potential. The effective two(three)-body interaction, then replaces the interaction term in H_A^Ω. We note that the effective interaction, by construction, converges to the original bare interaction as the basis space is increased and, thus, the NCSM calculation converges to the exact solution with the basis-space enlargement. In fact, it converges much faster than the corresponding bare interaction calculation performed in the same basis. Eventually, the A-nucleon P-space calculation can be performed either in a Slater-determinant single-particle HO basis or in a properly antisymmetrized Jacobi-coordinate HO basis. The latter is used in the present ^{4}He calculation. In the past, we applied this approach successfully to the ^{4}He interacting by the CD-Bonn NN potential. It turns out that the convergence with the AV8′ is significantly slower. The limitation to a two-body effective interaction is inadequate in the P spaces that we could access ($N_{\max}=18$). Therefore, we performed the calculations using the three-body effective interaction. The mean values of the different operators were calculated using the corresponding effective operators computed within the Lee-Suzuki approach in a two-body approximation using the formula derived in Ref. [47].

G. Effective interaction hyperspherical harmonic method

Similarly to the preceding method the EIHH approach introduces a two-body effective interaction V_{eff} [48]. The division of the total HH space in P and Q spaces is realized via the HH quantum number K [$P(Q)$ space: $K\leqslant(>)K_{\max}$]. Two powerful algorithms recently developed for the construction of symmetrized HH functions are employed [50,51]. In hyperspherical coordinates the total Hamiltonian is written as

$$H=\frac{1}{2m}\left(-\Delta_\rho+\frac{\hat{K}^2}{\rho^2}\right)+\sum_{i<j}V_{ij}, \tag{21}$$

where ρ is the hyper-radius and Δ_ρ contains derivatives with respect to ρ only. The grand-angular momentum operator $\hat{K}^2$ is a function of the variables of particles A and $(A-1)$ and of $\hat{K}_{A-2}$ the grand angular momentum operator of the $(A-2)$ residual system [52]. Then from the total Hamiltonian one can extract a ''two-body'' Hamiltonian of particles A and $(A-1)$

$$H_2(\rho)=\frac{1}{2m}\frac{\hat{K}^2}{\rho^2}+V_{A(A-1)}, \tag{22}$$

which, however, contains the hyperspherical part of the total kinetic energy. Since the HH functions of the $(A-2)$ system are eigenfunctions of $\hat{K}^2_{A-2}$ one has an explicit dependence of H_2 on the quantum number K_{A-2} of the residual system, i.e., $H_2\rightarrow H_2^{K_{A-2}}$. Applying the Hermitian version of the Lee-Suzuki method [46] to H_2 one gets an effective Hamiltonian H_{2eff}. The effective interaction V_{eff} is obtained from

$$V_{eff}^{K_{A-2}}(\rho)=H_{2eff}^{K_{A-2}}(\rho)-\frac{1}{2m}\frac{\hat{K}^2}{\rho^2}. \tag{23}$$

This V_{eff} replaces V_{ij} in Eq. (21) when we project the solution on the P space. This effective potential has the following property: $V_{eff}\rightarrow V_{ij}$ for $P\rightarrow 1$. Due to the ''effectiveness'' of the operator the solution of the Schrödinger equation converges faster to the true one. The HH formulation leads to various advantages: (i) V_{eff} itself is ρ dependent, therefore it contains some information on the ''medium,'' (ii) because of the above mentioned K_{A-2} dependence the (A-2) residual system is not a pure spectator, and (iii) an additional confining potential is not needed, since the presence of ρ in Eq. (22) automatically confines the two-body system to the range $0\leqslant r_{A-(A-1)}<\sqrt{2}\rho$. We would like to point out that $V_{eff}(K_{\max})$ can be viewed as a kind of momentum expansion, since the short range resolution is increased with growing $K_{\max}$. As discussed for the NCSM approach one obtains a better convergence for the calculation of mean values introducing corresponding effective operators. Of course for the calculation of the mean value of the Hamiltonian, i.e., E_b, one already makes use of an effective operator, namely $H_{2eff}^{K_{A-2}}$.

III. RESULTS

The AV8′ interaction appears to be an ideal test potential to compare the different calculational schemes. It is derived from the realistic AV18 interaction [8] by neglecting the charge dependence and the terms proportional to L^2 and $(L\cdot S)^2$. Furthermore, in this work we omit the electromagnetic part of the interaction. The potential is local and its spin and isospin dependences are represented by operators. Because of its form it is tractable for all of the calculational schemes described above.

The potential consists of eight parts:

$$\begin{aligned}V(r)&=V_c(r)+V_\tau(r)(\tau\cdot\tau)+V_\sigma(r)(\sigma\cdot\sigma)\\&\quad+V_{\sigma\tau}(r)(\sigma\cdot\sigma)(\tau\cdot\tau)+V_t(r)S_{12}+V_{t\tau}(r)S_{12}(\tau\cdot\tau)\\&\quad+V_b(r)(L\cdot S)+V_{b\tau}(r)(L\cdot S)(\tau\cdot\tau)\\&=\sum_{i=1}^{8}V_i(r)\mathcal{O}_i,\end{aligned} \tag{24}$$

where $(\sigma\cdot\sigma),(\tau\cdot\tau),S_{12}$, and $(L\cdot S)$ stand for spin-spin, isospin-isospin, tensor, and spin-orbit interactions [8], respectively, and $V_i(r)$ are radial functions of Yukawa- and Woods-Saxon types. The AV18 and AV8′ are defined with $\hbar^2/m_N=41.47108$ MeV fm^2, computed from the average of the proton and neutron masses. Most of the results reported here were obtained using the traditional value of 41.47; this results in a change in $\langle H\rangle$ of only $\approx$2.6 keV, far less than the estimated errors in the various methods.

First, we compare the binding energy results E_b, the expectation values of the kinetic and potential energy and the radii in Table I. We find good agreement for E_b within 3 digits or within 0.5%. This is quite remarkable in view of the

TABLE I. The expectation values $\langle T\rangle$ and $\langle V\rangle$ of kinetic and potential energies, the binding energies E_b in MeV, and the radius in fm.

Method	$\langle T\rangle$	$\langle V\rangle$	E_b	$\sqrt{\langle r^2\rangle}$
FY	102.39(5)	−128.33(10)	−25.94(5)	1.485(3)
CRCGV	102.30	−128.20	−25.90	1.482
SVM	102.35	−128.27	−25.92	1.486
HH	102.44	−128.34	−25.90(1)	1.483
GFMC	102.3(1.0)	−128.25(1.0)	−25.93(2)	1.490(5)
NCSM	103.35	−129.45	−25.80(20)	1.485
EIHH	100.8(9)	−126.7(9)	−25.944(10)	1.486

very different techniques and the complexity of the nuclear force chosen. Except for NCSM and EIHH, the expectation values of T and V also agree within three digits. The NCSM results are, however, still within 1% and EIHH within 1.5% of the others, but note that the EIHH results for T and V are obtained with bare operators. The uncertainty in the NCSM results is of the same size, i.e., 1 MeV, as that for the GFMC. Finally, the given radii are also in very good agreement.

The HH calculation includes about 4500 states with $\mathcal{L}=l_1+l_2+l_3\leqslant 6$. The states with $\mathcal{L}=6$ give a contribution to the binding energy of approximately 0.04 MeV. It is to be noticed that the HH spin-isospin states $\Phi_\mu^{(H)}$ having $\mathcal{L}\leqslant 6$ but constructed with the H-type Jacobi coordinates are linearly dependent on those considered in the expansion and therefore it is unnecessary to include them. The contribution of $\Phi_\mu^{(K)}$ (and $\Phi_\mu^{(H)}$) to the binding energy with $\mathcal{L}\geqslant 8$ has been estimated to be approximately 0.01 MeV.

The errors quoted for the GFMC results are just the Monte Carlo statistical errors. Various tests show that the energy is converged to at least this accuracy for changes in $\Delta\tau$ or the maximum τ. There should be no other sources of systematic error in this simple test case.

The NCSM binding energy result is based on extrapolation from calculations using the three-body effective interaction in model spaces up to $N_{\max}=16$ in the HO frequency range $\hbar\Omega=16-43$ MeV. The mean values of different operators, evaluated for $N_{\max}=16$ consisting of 2775 basis states and $\hbar\Omega=28$ MeV, were computed using effective operators as the use of bare operators is completely insufficient, in particular for the $V_c(r)$ and T. Note that we have here $\langle T_{\rm eff}\rangle+\langle V_{\rm eff}\rangle$ close, but not exactly equal to $\langle H_{\rm eff}\rangle$, due to approximations used. Overall, the NCSM results are less accurate than the other methods. The NCSM convergence rate is rather slow for the AV8′. However, the method is flexible to handle also nonlocal realistic potentials like the CD-Bonn with a faster convergence rate due to a softer repulsive core. The advantage of the method is its applicability to the p-shell nuclei.

The EIHH calculation is carried out with $K_{\max}=20$ (about 3000 HH states). The error estimate is based on the convergence with respect to $K_{\max}$, i.e., difference of results for $K_{\max}=18$ and 20. An inspection of Table I shows that E_b and radius are converged to a very high precision (E_b: 0.04%; radius: 0.007%, not shown in Table I). On the contrary $\langle T\rangle$ and $\langle V\rangle$ still change by about 1% from $K_{\max}=18$ to $K_{\max}=20$. Of course, by construction of the EIHH method, also $\langle T\rangle$ and $\langle V\rangle$ have to converge to the true result. In order to have a higher precision one can proceed in two ways: (i) increase of $K_{\max}$, (ii) use of effective operators. Particularly advantageous is the use of effective operators, since it allows us to make rather precise calculations with a small number of basis functions (see discussion of EIHH result for Fig. 1). As Table I shows it is not necessary to use effective operators for long-range observables like the radius, while observables that contain short range information (high momentum contributions), like $\langle T\rangle$ and $\langle V\rangle$, should, in principle, be calculated with effective operators.

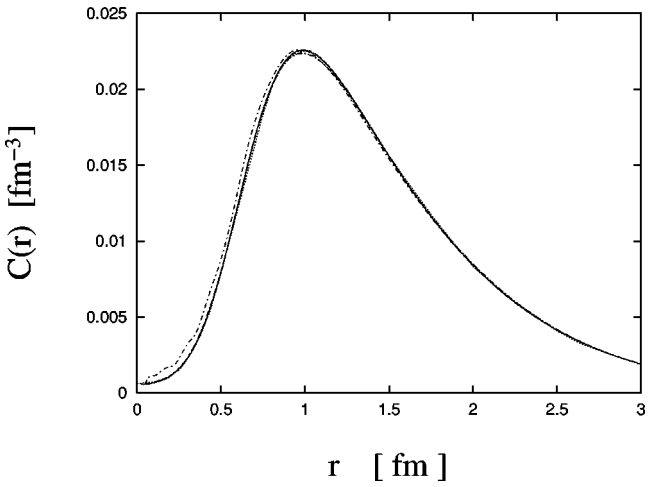

FIG. 1. Correlation functions in the different calculational schemes: EIHH (dashed-dotted curves), FY, CRCGV, SVM, HH, and NCSM (overlapping curves).

A more detailed test of the wave function is to evaluate the expectation values of the eight individual potential energy operators in Eq. (24). The results are shown in Table II. The agreement is, in general, rather good and well within

TABLE II. Expectation values of the eight potential operators in Eq. (24) in MeV.

Method	$\langle V_c\rangle$	$\langle V_\tau\rangle$	$\langle V_\sigma\rangle$	$\langle V_{\sigma\tau}\rangle$
FY	16.54	−5.038	−9.217	−57.55
CRCGV	16.54	−5.035	−9.215	−57.51
SVM	16.54	−5.036	−9.213	−57.51
HH	16.57	−5.034	−9.255	−57.59
GFMC	16.5(5)	−5.03(6)	−9.21(7)	−57.3(5)
NCSM	16.16	−4.92	−9.77	−57.89

Method	$\langle V_t\rangle$	$\langle V_{t\tau}\rangle$	$\langle V_b\rangle$	$\langle V_{b\tau}\rangle$
FY	0.707	−69.06	10.79	−15.50
CRCGV	0.708	−68.99	10.60	−15.30
SVM	0.707	−69.03	10.78	−15.49
HH	0.702	−69.03	10.76	−15.46
GFMC	0.71(3)	−68.8(5)	10.62(15)	−15.40(15)
NCSM	0.68	−69.13	11.23	−15.80

TABLE III. Expectation values of potential energy operators in MeV.

Method	Central	Tensor	Spin-orbital
FY	−55.26	−68.35	−4.72
CRCGV	−55.22	−68.28	−4.70
SVM	−55.23	−68.32	−4.71
HH	−55.31	−68.32	−4.71
GFMC	−55.05(70)	−68.05(70)	−4.75(5)
NCSM	−56.43	−68.45	−4.57

TABLE IV. Probabilities of total orbital angular momentum components in %.

Method	*S* wave	*P* wave	*D* wave
FY	85.71	0.38	13.91
CRCGV	85.73	0.37	13.90
SVM	85.72	0.368	13.91
HH	85.72	0.369	13.91
NCSM	86.73	0.29	12.98
EIHH	85.73(2)	0.370(1)	13.89(1)

1%, except for NCSM with discrepancies up to 6% but they are generally 4% or less. In the case of the CRCGV, the expectation values for the spin-orbit operators are a bit off from the rest, but again still within 4%. There are no results given for the EIHH.

Table III shows the expectation values of the sum of the first four operators in Eq. (24) (called central), of the two tensor operators and of the two spin-orbit operators. Again, no results are given for the EIHH. Except for the NCSM with differences up to 3.2%, all the values agree quite well each other.

As a further property of the wave function we consider the *NN* correlation function

$$C(r)=\langle\Psi|\,\delta(\vec{r}-\vec{r}_{12})|\Psi\rangle, \tag{25}$$

where $\vec{r}_{12}=\vec{r}_1-\vec{r}_2$. It is apparently normalized as $4\pi\int C(r)r^2dr=1$. The results for the various calculational schemes, except for the GFMC are shown in Fig. 1. The agreement among the FY, CRCGV, SVM, HH, and NCSM is essentially perfect. For the EIHH it is necessary to use an effective operator in order to obtain good convergence also for $r<1.2$ fm. Due to the use of rather unsophisticated computers, the EIHH calculation for $C(r)$ is performed with the rather low $K_{\max}$ value of 12 (about 400 HH states); however, a rather good agreement with the other methods is already obtained at this low value.

Finally, we show in Table IV the probabilities for finding the three different total orbital angular momenta in our $4N$ model system. The agreement among the different methods is very good with a small excursion in NCSM.

To summarize, we have demonstrated that the Schrödinger equation for a four-nucleon system can be handled quite reliably by different methods leading to very good agreement in the binding energy, in expectation values of the kinetic and potential energies and in simple wave function properties. The AV8′ *NN* potential encompasses most of the complexity of realistic *NN* forces and, thus, the benchmark calculations are highly nontrivial and demonstrate the maturity and reliability of various methods. These results are good foundations for further investigations of nuclear structure for more complex systems and/or for other *NN* interaction models.

We have chosen the AV8′ potential because it can be handled without any approximation by all of our methods. More realistic *NN* potentials such as AV18 [8], CD-Bonn [7], and Nijmegen I,II [9] pose additional difficulties for at least some of the methods. There are new operator forms with higher order derivatives or very strong nonlocalities. Also some of the potentials are defined partial wave by partial wave.

Whereas in the four-body system the FY and NCSM schemes can handle all types of *NN* potentials directly, the GFMC method relies on AV8′ and treats the difference to AV18 in perturbation theory. The SVM can in principle treat any local potential, such as AV18, but the $(L\cdot S)^2$ terms require additional computational effort. Also the remaining methods, HH, CRCGV, and EIHH, can handle more complicated potentials, although at present applications have been restricted to local potentials. GFMC, NCSM, SVM, and EIHH have already obtained solutions for $A>4$, whereas FY up to now has been restricted to $A\leqslant 4$. An advantage of the methods, CRCGV and EIHH, is that they do not need as heavy computational facilities as the other methods.

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