Variational calculations with correlated basis functions: Three-nucleon and three-alpha-particle systems

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A new variational method is applied to the solution of the Schrödinger equation for interacting few-body systems. The results for three nucleons interacting via the spin-dependent Malfliet-Tjon potential and three alpha particles interacting via the Ali-Bodmer potential are presented and compared with Faddeev and amalgamation of two-nucleon correlations in multiple scattering process results, respectively.

In a previous paper[1] a new complete basis of wave functions for the treatment of interacting few-body systems has been introduced with the aim of improving the existing variational-type calculations, particularly the ones based upon the expansion of the bound states onto the harmonic-oscillator basis[2] [variational harmonic oscillator (VHO) method]. As a matter of fact, even with simple interactions, like, e.g., the central nucleon-nucleon potentials, it turned out that, (i) the convergence of the ground-state energy can be reached only by using a high number of basis states (see Ref. 1), (ii) the convergence of the energy is no guarantee that other quantities converge as well (see Ref. 3), and (iii) VHO wave functions have a wrong asymptotic behavior at large interparticle distances, which is the reason for the observed poor convergence of the momentum distribution at low momenta (see Ref. 4).

As explained in Ref. 1, the new variational method [hereafter called the correlated VHO (CVHO) method] is based upon the expansion of few-body bound states onto a complete set of properly correlated basis states obtained by multiplying the usual HO wave functions by a scalar symmetric correlation factor of the Jastrow form:

$$F=\prod_{i<j} f(|\mathbf{r}_i-\mathbf{r}_j|) \ . \tag{1}$$

It can be seen that the VHO method is recovered when $F=1$.

The CVHO method was successfully applied[1] to three nucleons interacting via central potentials. It turned out that the introduction of the correlation factor F drastically improved the convergence of the triton static properties as well as the tail of the one-body and two-body distribution functions.

In this Brief Report both the results obtained for three nucleons interacting via the spin-dependent Malfliet-Tjon potential MT/I-III,[5] acting only in the s wave, and those for three alpha particles interacting via the central Ali-Bodmer potential d_0,[6] acting in all partial waves, will be presented and compared with the available results based on the amalgamation of two-nucleon correlations in multiple scattering process (ATMS) approach[7] and configuration space Faddeev (FCS) calculations.[8]

For pure S-wave ground states the CVHO trial wave function is written in the form[1]

$$\Psi=F\left[\sum_{k=1}^{N} b_k\Phi_k^{\mathrm{HO}}(\mathbf{x},\mathbf{y})\right]\cdot\chi \ , \tag{2}$$

where χ is the appropriate spin factor, $\Phi_k^{\mathrm{HO}}(\mathbf{x},\mathbf{y})$ is an S-wave HO function expressed in terms of intrinsic coordinates

$$\{\mathbf{x}=\mathbf{r}_1-\mathbf{r}_2,\ \mathbf{y}=2[\mathbf{r}_3-(\mathbf{r}_1+\mathbf{r}_2)/2]/3\} \ ;$$

k stands for $\{n_x,n_y,l_x,l_y\}$ where n and l are radial and orbital quantum numbers; N is the number of HO states corresponding to excitation quanta

$$Q<Q_0=2n_x+2n_y+l_x+l_y$$

with $l_x=l_y$; finally, F is the correlation factor of Eq. (1). The two-body correlation function $f(|\mathbf{r}_i-\mathbf{r}_j|)=f(r)$ used in the calculations is

$$f(r)=\{[1-\epsilon_1 e^{-(r/b_1)^{n_1}}][1+\epsilon_2(r/b_2)^{n_2}e^{-(r/b_2)^2}]\}^{1/2} \tag{3}$$

for the 3-α system and

$$f(r)=(1-\epsilon_1' e^{-(r/b_1')^2}-\epsilon_2' e^{-(r/b_2')^2})^{1/2} \tag{4}$$

for the three-nucleon system.

The results obtained with the VHO and CVHO methods, reported in Tables I and II, clearly show that the rate of convergence of the calculated quantities is drastically improved by the CVHO method.

For the 3-α system (see Table I), the CVHO method yields 99.9% of the final value of the energy already with $Q_0=8$ (22 basis states), whereas with the VHO method the same energy is obtained only when $Q_0=32$ (525 basis states). The agreement between the ATMS and CVHO results is excellent. In Fig. 1 the charge form factors calculated by the VHO, CVHO, and ATMS methods are compared. It clearly appears that for the 3-α system (with the Ali-Bodmer potential) the VHO, CVHO, and ATMS methods yield very similar results. However, we would like to stress that, (i) in the CVHO method it is sufficient to consider 8 excitation quanta only, whereas in the VHO method one has to use 32 excitation quanta, and (ii) the CVHO method can be applied even for potentials acting in a finite number of partial waves, whereas in the ATMS method the treatment of such a case seems to be a very difficult task.

For the three-nucleon system the improvement of the convergence is more remarkable than for the 3-α system. From Table II it can be seen that the CVHO method yields 99.5% of the final values of the computed quantities at

TABLE I. 3-α system: ground-state energy (B), mean kinetic energy ($\langle T\rangle$), mass radius (R_m) and the form factor evaluated at $q=2.0$ fm^{-1} ($|F_{\max}|$) calculated by the VHO and CVHO methods with the Ali-Bodmer potential d_0 (Ref. 6) (acting in all partial waves) for various values of the number of oscillator quanta Q_0. For the VHO basis the value of the harmonic-oscillator (HO) length is $a=2.00$ fm, which corresponds to the best variational energy at $Q_0=20$. The variational parameters [the HO length and the correlation function parameters appearing in Eq. (3)] used in the CVHO basis are $a=2.54$ fm, $\epsilon_1=1.00$, $b_1=2.25$ fm, $n_1=4.49$, $\epsilon_2=2.57$, $b_2=2.00$ fm, $n_2=3.03$. These values have been obtained by minimizing the variational energy at $Q_0=8$. The results obtained by the ATMS method (Ref. 7) are also reported.

	VHO basis					CVHO basis			
Q_0	B (MeV)	$\langle T\rangle$ (MeV)	R_m (fm)	$\lvert F_{\max}\rvert$ $\times 10^{-2}$	Q_0	B (MeV)	$\langle T\rangle$ (MeV)	R_m (fm)	$\lvert F_{\max}\rvert$ $\times 10^{-2}$
0	153.70	7.78	1.41	26.4	0	5.62	11.35	1.88	0.4
4	−1.61	8.42	2.23	9.5	2	−3.19	7.47	2.33	4.1
8	−3.70	6.30	2.46	6.3	4	−4.88	7.05	2.43	7.9
12	−4.66	7.21	2.45	6.8	6	−5.14	7.62	2.42	6.3
16	−5.06	7.53	2.44	6.5	8	−5.17	7.70	2.43	6.4
20	−5.13	7.53	2.44	6.4	10	−5.18	7.70	2.43	6.4
24	−5.14	7.56	2.44	6.4	12	−5.18	7.70	2.43	6.4
28	−5.16	7.62	2.44	6.4					
32	−5.17	7.66	2.43	6.4					
				ATMS (Ref. 7)					
	−5.18	7.71	2.43	6.4		−5.18	7.71	2.43	6.4

$Q_0=10$ (56 basis states), while in the VHO method the convergence is far from being reached even at $Q_0=26$ (560 basis states); in particular, 11% of the energy and 22% of the mixed-symmetry S-wave probability ($P_{S'}$) are still missing at $Q_0=26$.

The agreement between the CVHO and FCS[8] results is excellent for the S'-wave probability and the charge radius of ^{3}H, whereas the binding energies differ by ~ 50 keV; since we are very confident in our extrapolated value, it would be very interesting to have an independent check of ^{3}H binding energy with the MT/I–III potential. From the results presented in Table II, it can also be seen that the ex-

TABLE II. Triton: ground-state energy (B), mean kinetic energy ($\langle T\rangle$), S'-wave probability ($P_{S'}$), point proton radius (R_p) and the momentum distribution $n(k)$ evaluated at $k=0$ calculated by the VHO and CVHO methods with the spin-dependent Malfliet-Tjon potential MT/I-III (acting in the s wave only) for various values of the number of oscillator quanta Q_0. For the VHO basis the value of the HO length is $a=1.20$ fm, which corresponds to the best variational energy at $Q_0=20$. The variational parameters [the HO length and the correlation function parameters appearing in Eq. (4)] are $a=2.46$ fm, $\epsilon_1'=4.43$, $b_1'=0.60$ fm, $\epsilon_2'=3.50$, $b_2'=1.81$ fm. These values correspond to the best variational energy at $Q_0=8$. The results based on the Faddeev theory (Ref. 8) (FCS) are also reported. Finally, the energy calculated at Q_0^∞ corresponds to the extrapolated value of $Q_0\to\infty$ according to the formula $B(Q_0)=B(Q_0^\infty)e^{-(\beta/Q_0)^\alpha}$.

	VHO basis					CVHO basis				
Q_0	B (MeV)	$\langle T\rangle$ (MeV)	$P_{S'}$ (%)	R_p (fm)	$n(k=0)$ (fm^3)	B (MeV)	$\langle T\rangle$ (MeV)	$P_{S'}$ (%)	R_p (fm)	$n(k=0)$ (fm^3)
0	91.64	86.40	0.0	0.84	3.90	−5.86	41.72	0.0	1.38	20.4
2	21.67	58.72	1.12	1.07	6.66	−7.81	30.69	1.69	1.53	27.0
4	12.27	48.55	0.94	1.19	8.77	−7.99	30.69	1.86	1.55	28.0
6	3.60	41.80	0.87	1.28	11.6	−8.35	29.99	1.94	1.59	33.7
8	0.37	38.77	0.94	1.33	13.5	−8.40	30.05	1.94	1.60	33.6
10	−2.27	36.28	0.99	1.38	15.9	−8.44	30.07	1.96	1.61	35.8
12	−3.87	34.95	1.06	1.42	17.7	−8.460	30.03	1.96	1.61	36.5
14	−4.98	33.85	1.14	1.44	19.5	−8.473	30.03	1.96	1.61	37.0
16	−5.78	33.16	1.22	1.47	21.1	−8.482	30.03	1.96	1.61	37.2
18	−6.36	32.54	1.29	1.50	22.7					
20	−6.80	32.14	1.36	1.51	24.0					
22	−7.12	31.79	1.42	1.52	25.3					
24	−7.38	31.52	1.48	1.53	26.4					
26	−7.57	31.31	1.53	1.54	27.4					
Q_0^∞	-8.5 ± 0.2					-8.50 ± 0.01				
					FCS (Ref.8)					
	−8.54		1.95	1.62		−8.54		1.95	1.62	

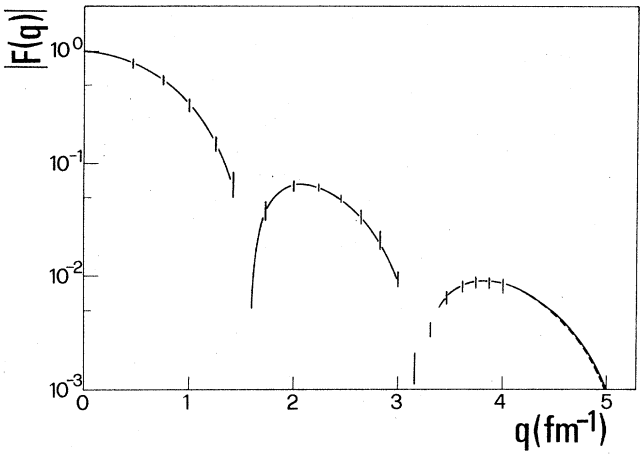

FIG. 1. Charge form factor of the 3-α system corresponding to the Ali-Bodmer potential d_0 acting in all partial waves. Dashed line, VHO method at $Q_0=32$ (525 basis states); full line, CVHO method at $Q_0=12$ (50 basis states); bars, ATMS method (Refs. 7 and 9).

trapolation of the calculated energy to $Q_0 \rightarrow \infty$ may not be very reliable in the VHO method.

In Fig. 2 the charge form factors of ^{3}H calculated by the VHO and CVHO methods are compared. In the same figure the convergence of the form factor evaluated at $q=5.2$ fm^{-1} and $q=8.6$ fm^{-1} is also shown. It can be seen that the convergence is completely reached only in the CVHO method. This is due to the improvement of the convergence of $P_{S'}$, since the S'-wave admixture greatly affects the elastic form factor as was explicitly shown in Ref. 2(a).

In Fig. 3 the point proton density of ^{3}H evaluated by the VHO and CVHO methods is shown. It turns out that the Gaussian decay of the VHO density starts already at $y\sim 3$ fm, whereas the CVHO density has the correct asymptotic behavior up to $y\sim 9$ fm. As a further test of the tail of our CVHO wave function, we have evaluated the momentum distribution $n(k)$ at $k=0$ (see Ref. 4).

From Table II it clearly appears that the convergence of $n(k=0)$ is reached only with the CVHO method.

In a previous paper[1] the CVHO method was used with pure central interactions and excellent agreement with Green's function Monte Carlo (GFMC), variational Jastrow Monte Carlo (VJM), and Faddeev (FCS) results were obtained. Also, recent ATMS calculations[10] for ^{3}H using the MT/V interaction[5] yield results in agreement with our CVHO method[1] (a thorough numerical comparison of the two methods is under investigation[11]). The results exhibited in this Brief Report show an agreement of the same quality with FCS and ATMS methods when spin-dependent N-N interaction and local α-α potential are used. It should, however, be pointed out that a very small but not negligible difference (up to ~ 200 keV) exists between the FCS and our energies when the N-N interaction acts only in the s wave for both central and spin-dependent potentials. Results for Reid soft-core potential and l-dependent α-α interaction will be published elsewhere.

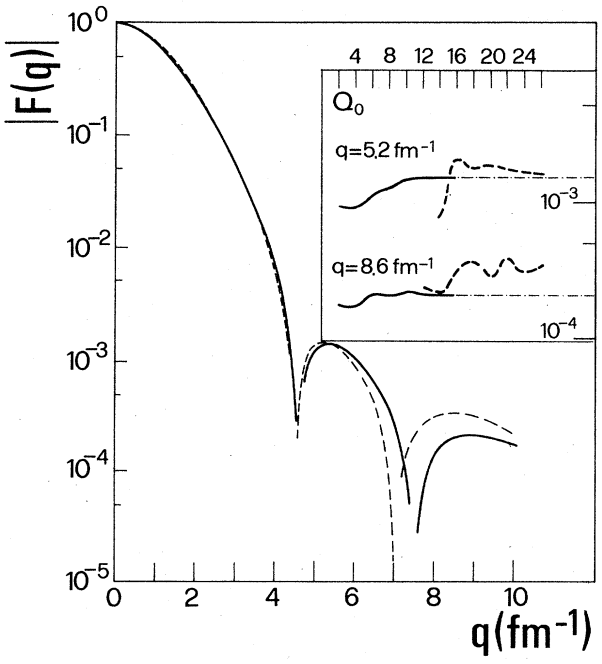

FIG. 2. Charge form factor of ^{3}H with the spin-dependent Malfliet-Tjon potential MT/I-III acting in the s wave only. Dashed line: VHO method at $Q_0=26$ (560 basis states). Full line, CVHO method at $Q_0=12$ (84 basis states). In the right upper corner the convergence of the form factor evaluated at $q=5.2$ fm^{-1} and $q=8.6$ fm^{-1} is reported. Dashed line, VHO method; full line, CVHO method.

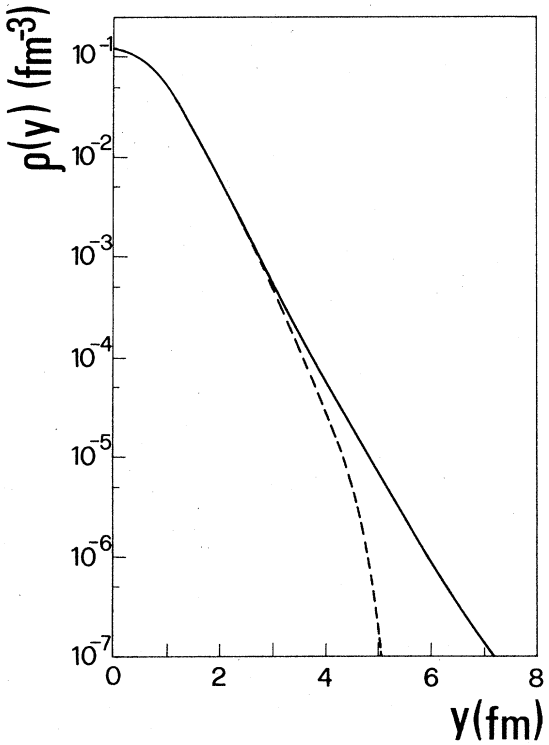

FIG. 3. Point proton density of ^{3}H with the MT/I-III potential acting only in the s wave. Dashed line, VHO method at $Q_0=26$; Full line, CVHO method at $Q_0=12$. Note that up to $y\sim 9$ fm the tail of the CVHO density is proportional to $e^{-2\gamma y}/y^2$ where $\gamma=(M|E_3|/\hbar^2)^{1/2}$ with E_3 being the calculated ground-state energy.

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