Variational calculation of the α particle with the Paris potential

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The ground state of the α particle is calculated using a revised version of the Brillouin-Wigner perturbation method, with enhanced variational flexibility. The resulting energy eigenvalue, for the Paris potential, is -25.5 MeV. When Coulomb forces and possible errors are taken into account one establishes an upper bound on the eigenvalue of -24.1 MeV. The derived wave function contains a D state admixture of only 5.36%.

I. INTRODUCTION

An important advantage of the Brillouin-Wigner[1,2] perturbation procedure lies in its variational properties. It is considerably more straightforward to judge the accuracy of an approximate energy eigenvalue if one knows that one has calculated an upper bound, and not overshot the exact result. Without a variational principle it could be extremely difficult to know if an extension to a higher order of approximation actually leads to an improvement.

When the eigenvalue is supported by an upper bound theorem one may attempt improvements by inserting additional variational flexibility into the trial wave function. The Brillouin-Wigner wave function has proven to be very accessible to such experiments.[3] Previous papers[4] have investigated a simple trial wave function, related to the Moszkowski-Scott[5] separation method, and designed for calculating the bound states of light nuclei with modern nuclear interaction operators.

The present paper extends this work in two respects. In Ref. 4 a Gaussian potential was fitted to the lowest Talmi integrals of the Reid[6] soft core potential, so that all the integrals could be performed in closed form. Thus the eigenvalue approximate obtained is not an upper bound for the Reid soft core potential; but it is for the simulated potential. In the present work the recent Paris interaction is used in its entirety, without any mutilation. Second, considerable new variational flexibility has been introduced into the trial wave function to improve the accuracy of the upper bound. This will be described more fully in Secs. II and III.

II. METHOD

The Hamiltonian is written in the form

$$H=H_0+W\ , \tag{1}$$

where

$$H_0=\tfrac{1}{2}\hbar\omega\sum_{i=1}^{A}(p_i^2+q_i^2)-U-\tfrac{3}{2}\hbar\omega \tag{2}$$

defines a set of (antisymmetrized) oscillator functions

$$H_0\varphi_n(1,\ldots,A)=\epsilon_n\varphi_n(1,\ldots,A) \tag{3}$$

and

$$W=\sum_{i<j}v_{ij}-\left[\frac{\hbar\omega}{2A}\right]\sum_{i<j}q_{ij}^2+U\ , \tag{4}$$

where v_{ij} is the two-body Paris interaction.

The variational trial wave function is chosen in the form:

$$\psi=\varphi_0+\sum_i K_i\sum_{n\neq 0}\frac{\varphi_n\langle n\mid W^i\mid 0\rangle}{E-\epsilon_n}\ . \tag{5}$$

In previous work[3,4] one maintained the condition $\sum W^i=W$. In the present example, however, this will not be the case. We reserve the right to select the W^i later to obtain more variational flexibility in ψ. This is clearly permissible, so long as one does not violate the boundary or symmetry conditions of the wave function.

Substituting Eq. (5) into the variational integral

$$E=\frac{\langle\psi\mid H\mid\psi\rangle}{\langle\psi\mid\psi\rangle} \tag{6}$$

one obtains

$$E=\epsilon_0+W_{00}+2\sum_i K_iE_2(i)+\sum_{i,j}K_iK_j[E^{(3)}(i,j)-E^{(2)}(i,j)]\ , \tag{7a}$$

where

$$E_2(i)=\sum_{n\neq 0}\frac{\langle 0\mid W\mid n\rangle\langle n\mid W^i\mid 0\rangle}{(E-\epsilon_n)}\ , \tag{7b}$$

$$E^{(2)}(i,j)=\sum_{n\neq 0}\frac{\langle 0\mid W^i\mid n\rangle\langle n\mid W^j\mid 0\rangle}{(E-\epsilon_n)}\ , \tag{7c}$$

and

$$E^{(3)}(i,j)=\sum_{n,m\neq 0}\frac{\langle 0\mid W^i\mid n\rangle\langle n\mid W\mid m\rangle\langle m\mid W^j\mid 0\rangle}{(E-\epsilon_n)(E-\epsilon_m)}\ . \tag{7d}$$

Variation of the K_i,

$$\frac{\partial E}{\partial K_i}=0\ , \tag{8}$$

to optimize the eigenvalue yields the set of equations

$$E_2(i)=\sum_j K_j[E^{(2)}(i,j)-E^{(3)}(i,j)] \ . \tag{9}$$

Substitution of Eq. (9) into Eq. (7) gives us

$$E=\epsilon_0+W_{00}+\sum_i K_i E_2(i) \ . \tag{10}$$

Now if one constructs column matrices E_2 and K out of the elements of $E_2(i)$ and K_i, respectively, and likewise square matrices $E^{(2)}$ and $E^{(3)}$ out of $E^{(2)}(i,j)$ and $E^{(3)}(i,j)$, then Eqs. (10) and (9) may be combined to eliminate K and yield a form most convenient to calculation:

$$E=\epsilon_0+W_{00}+\tilde{E}_2[E^{(2)}-E^{(3)}]^{-1}E_2 \ . \tag{11}$$

III. DETAILS OF THE TRIAL WAVE FUNCTION

If one chooses to partition the W^i such that $\sum W^i=W$ in the preceding section then one has precisely the method in Ref. 4. For modern nuclear forces this will lead us to some rather formidable eightfold integrals which must be done by strictly numerical methods. Clearly there is no reason to attempt to deal with such complications. One still retains a broad choice in selecting the W^i. This choice is to be guided by two criteria. First, one should have mathematical problems which are conveniently disposed of on modern computers. Second, one should produce a reasonably accurate wave function.

The choice to be tested in this paper can be written in three parts

$$W^i(^3S_1)=\sum_{j<k}\hbar\omega P_0(j,k)\exp(-\alpha_i q_{jk}^2) \ , \tag{12}$$

$$W^i(^1S_0)=\sum_{j<k}\hbar\omega P_1(j,k)\exp(-\alpha_i q_{jk}^2) \ , \tag{13}$$

and

$$W^i(D)=-\sum_{j<k}\hbar\omega S_{jk}q_{jk}^2\exp(-\alpha_i q_{jk}^2) \ . \tag{14}$$

Here P_0 and P_1 are projection operators for the $T=0$, $S=1$ and the $T=1$, $S=0$ states, respectively:

$$P_0(j,k)=\tfrac{1}{16}(3+\vec{\sigma}_j\cdot\vec{\sigma}_k)(1-\vec{\tau}_j\cdot\vec{\tau}_k) \ , \tag{15}$$

$$P_1(j,k)=\tfrac{1}{16}(1-\vec{\sigma}_j\cdot\vec{\sigma}_j)(3+\vec{\tau}_j\cdot\vec{\tau}_k) \ , \tag{16}$$

and S_{jk} is the usual tensor operator

$$S_{jk}=3\vec{\sigma}_j\cdot\hat{n}\,\vec{\sigma}_k\cdot\hat{n}-\vec{\sigma}_j\cdot\vec{\sigma}_k \ . \tag{17}$$

Thus one forms a perturbed defect function for each two-body channel available in ^{4}He.

The α_i represent some grid of numbers. Ideally they could be varied to minimize the upper bound. Since the final expression for the eigenvalue is not linear in the α_i, this is a rather time consuming procedure. A better alternative presents itself after one has looked at the basic expressions involved.

Most of the procedures and equations of Ref. 4 are now directly applied to the present α-particle calculation. The *only* difference in procedure is that previously the nuclear interaction was taken to be a linear combination of Gaussians, so that all of the integrations could be performed in closed form, while in the present work with the Paris potential many of these integrals must be done by numerical methods. Let us now display these integrals.

First, in order to clarify the notation, note that the integrals needed to calculate $E^{(2)}$ are the same as those given in Ref. 4, for example,

$$\left[z_{ij}^{\alpha}\frac{1}{e}z_{ij}^{\alpha'}\right]_{00}=-\hbar\omega(1-\beta)^{3/2}(1-\beta')^{3/2}\int_0^1 t^{\delta-1}[1-n_0\beta\beta' t^2]^{-3/2}dt \ , \tag{18}$$

where

$$\beta=\alpha/(1=\alpha),$$

$$-\hbar\omega\delta=E-\epsilon_0 \ ,$$

$$e=E-H_0 \ ,$$

and

$$z_{ij}^{\alpha}=\hbar\omega\exp(-\alpha q_{ij}^2) \ . \tag{19}$$

The parameter n_0 depends on the partition of particle labels (ij,kl), and are specified in Table I. The matrix element becomes[4]

$$\left[z_{ij}^{\alpha}\frac{Q}{e}z_{kl}^{\alpha'}\right]_{00}=\left[z_{ij}^{\alpha}\frac{1}{e}z_{kl}^{\alpha'}\right]_{00}+(\hbar\omega\delta)^{-1}(z_{ij}^{\alpha})_{00}(z_{ij}^{\alpha'})_{00} \tag{20}$$

after correction for the Pauli operator $Q=1-|0\rangle\langle 0|$.

The integrals needed for the central terms in E_2 are of the form:

$$\left[z_{ij}^{\alpha}\frac{1}{e}v_{kl}\right]_{00}=\pi^{-3/2}(1-\beta)^{3/2}\int_0^1 t^{\delta-1}(1-n_0\beta t^2)^{-3/2}dt\int v(q)\exp\left[\frac{-q^2}{1-n_0\beta t^2}\right]d\vec{\mathrm{q}} \ , \tag{21}$$

where $v(q)$ is the appropriate component of the Paris potential. To calculate $E^{(3)}$ one needs integrals of the form:

$$\left[z_{ij}^{\alpha}\frac{1}{e}v_{kl}\frac{1}{e}z_{mn}^{\alpha'}\right]_{00}=[\pi^{-1}(1-\beta)(1-\beta')]^{3/2}\int_0^1\int_0^1(t\tau)^{\delta-1}\Gamma_1^{-3/2}dt\,d\tau\int v(q)\exp[-\Gamma_2 q^2/\Gamma_1]d\vec{q}\ , \tag{22}$$

where

$$\Gamma_1=1-n_1\beta t^2-n_2\beta'\tau^2-n_4\beta\beta' t^2\tau^2\ , \tag{23}$$

$$\Gamma_2=1-n_3\beta\beta' t^2\tau^2\ , \tag{24}$$

and the n_i are given in Table I. Pauli corrected integrals for $E^{(3)}$ are

$$\left[z_{ij}^{\alpha}\frac{Q}{e}v_{kl}\frac{Q}{e}z_{mn}^{\alpha'}\right]_{00}=\left[z_{ij}^{\alpha}\frac{1}{e}v_{kl}\frac{1}{e}z_{mn}^{\alpha'}\right]_{00}+(\hbar\omega\delta)^{-1}(z_{ij}^{\alpha})_{00}\left[v_{kl}\frac{1}{e}z_{mn}^{\alpha'}\right]_{00}$$
$$+(\hbar\omega\delta)^{-1}(z_{mn}^{\alpha'})_{00}\left[z_{ij}^{\alpha}\frac{1}{e}v_{kl}\right]_{00}+(\hbar\omega\delta)^{-2}(z_{ij}^{\alpha})_{00}(v_{kl})_{00}(z_{mn}^{\alpha'})_{00}\ . \tag{25}$$

It should be noted that several of the above terms, like

$$\left[z_{12}^{\alpha}\frac{Q}{e}v_{34}\right]_{00}\ , \tag{26}$$

vanish identically due to the Pauli correction. The momentum dependent terms in the Paris potential cause no great problem, as one simply performs the indicated differentiations with respect to q within the integrands before performing the integrations. Likewise the tensor terms yield simple modifications in the integrands. The appropriate coefficients can be found in Ref. 4, where the $\vec{q}$ integration was carried out using Gaussian functions for v.

Thus by using Gaussian functions in the W^i one has only double integrals to deal with in E_2 and triple integrals in $E^{(3)}$. Actually the situation is not even that complicated. At least one of the integrations can always be reduced to an error function, and error functions present a trivial computational problem. The remaining single and double integrals were performed to a tolerance of 1 keV.

TABLE I. The n_i needed to calculate $E^{(2)}$, $E^{(3)}$, and E_2.

	(ij,kl)			n_0
	(12,12)			1
	(12,13)			$\frac{1}{4}$
	(12,34)			0
(ij,kl,mn)	n_1	n_2	n_3	n_4
(12,12,12)	1	1	1	−1
(12,12,13)	1	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
(12,13,12)	$\frac{1}{4}$	$\frac{1}{4}$	1	$\frac{1}{2}$
(12,13,23)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{2}$
(12,34,12)	0	0	1	1
(12,13,14)	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0
(12,12,34)	1	0	0	0
(12,13,34)	$\frac{1}{4}$	$\frac{1}{4}$	0	0
(12,34,13)	0	$\frac{1}{4}$	$\frac{1}{4}$	$-\frac{1}{4}$
(12,13,24)	0	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$

One must now select an appropriate grid of values for the α_i in the calculation. The selection is facilitated by considering the variable change

$$\beta_i\equiv\alpha_i(1+\alpha_i)^{-1}\ .$$

The dependence of the $E_2(i)$ in β_i is displayed in Table II. This is the final set used in the ^{4}He calculation reported in Sec. IV of this paper, with oscillator size parameter $b=1.6$ (10^{-13}) cm, and U iterated[4] so that $\delta=1$. There are two interesting points concerning these numbers.

First, note the surprisingly moderate variation of $E_2(i)$ with β_i over the full range of values $0\le\beta_i\le i$. This is particularly striking in the central contributions, $E_2(^3S_1,\beta_i)$ and $E_2(^1S_0,\beta_i)$, which must identically vanish at the end positions $\beta=0$ or 1. The tensor term $E_2(D,\beta_i)$ shows somewhat more variation with β_i. This is in part because $W^i(D)$ in Eq. (14) was chosen so that $E_2(D,\beta_i=0)$ does not vanish while $E_2(D,\beta_i=1)\equiv 0$. The figures in Table II imply that one does not need a very extensive grid of values for the β_i in the trial wave function in order to obtain a reasonable energy eigenvalue. Consequently only the values $\beta_i=0.1$, 0.3, 0.5, 0.7, and 0.9 were used in the calculation reported in Sec. IV.

The second point worthy of note in Table II is the relative size of the two-body and three-body contributions. The three-body terms are by no means small. This is basically due to the fact that there are so many of them. There are twenty-four terms of the type $[z_{12}(Q/e)v_{13}]_{00}$ against only six two-body terms of the type $[z_{12}(Q/e)v_{12}]_{00}$. The fact that the three-body contribution is larger in magnitude than the two body in the $^1S_0$ channel for small β_i is actually due to cross terms of $z(^1S_0,\beta_i)$ with the strong $^3S_1$ interaction of the Paris potential

$$[z_{12}(^1S_0,\beta_i)\frac{Q}{e}v_{13}(^3S_1)]_{00}\ . \tag{27}$$

Let us take an overall view of the interpretation of the trial wave function. For small values of β_i (say 0.1), the defect function contribution

$$\chi_i=K_i\sum_{n\neq 0}\frac{\varphi_n\langle n\mid W^i\mid 0\rangle}{E-\epsilon_n} \tag{28}$$

TABLE II. Comparison of two- and three-body contributions to $E_2(i)$ in MeV. All entries are corrected for the Pauli operator. The central terms include both momentum independent and dependent components of the Paris potential, and the oscillator potential correction (q_{ij}^2) in Eq. (4).

Type of term	β_i	Two-body part E_2	Three-body part E_2	Total $E_2(i)$
$W^i(^3S_1)$	0.1	−3.263	−1.972	−5.235
of Eq. (12)	0.3	−8.049	−4.214	−12.263
	0.5	−10.344	−4.410	−14.754
	0.7	−9.725	−2.998	−12.723
	0.9	−5.118	−0.773	−5.891
$W^i(^1S_0)$	0.1	−1.700	−2.734	−4.434
of Eq. (13)	0.3	−4.245	−5.792	−10.037
	0.5	−5.598	−6.060	−11.658
	0.7	−5.429	−4.120	−9.549
	0.9	−3.084	−1.067	−4.151
$W^i(D)$	0.1	−16.556	7.330	−9.226
of Eq. (14)	0.3	−10.008	3.295	−6.713
	0.5	−5.026	1.104	−3.922
	0.7	−1.700	0.202	−1.498
	0.9	−0.137	0.005	−0.132

will converge very rapidly as increasing n induces increasing quanta of the oscillator orbitals into the perturbed wave function. Thus, as this term emphasizes excitations of low energy (hence low momentum), its influence tends to come from the longer range components of the nuclear interaction. Conversely, for β near one (say 0.9) the series in Eq. (28) will converge very slowly with increasing n, thus mixing states of very high momentum into the wave function. This term must obtain its influence from the shorter range components of the nuclear interaction.

One sees, therefore, that this variational trial wave function accomplishes a separation in the effects of the long and short range components of the nuclear force. It is very similar to the philosophy of the Moszkowski-Scott[5] method, even though the mathematical details are very different.

If one were to partition the trial wave function into an unlimited number of terms (β_i), thereby using all the degrees of freedom of the excited configurations, one would attain a complete analysis of all two particle excitations out of the oscillator ground state. The objective of the present procedure, however, is to attempt an adequate representation of the true eigenstate with only a moderately sized partition.

IV. RESULTS

The values obtained for the K_i in each channel by solving Eq. (9) are shown in Table III. The corresponding energy eigenvalue for the α particle is −25.5 MeV. Coulomb interaction was not included in this calculation. It is not really hard to incorporate, but it is a nuisance to separate off the proton-proton channel in the isospin formalism. When one is finished with the rest of the calculation, however, one has a trial function with which one can readily estimate the Coulomb contribution to the energy to be 0.9 MeV. Since one has two contributions to the energy and both expectation values are calculated with the same trial function, it is legitimate to add them, and obtain an upper bound of −24.6 MeV.

There is one more correction to be considered before one can quote a rigorous upper bound. That is the numerical error accumulated in the calculation itself. There are three possible sources of error to be considered: (i) Not all of the parameters of the Paris potential[7] are given explicitly in the literature. Some are given by formulae, and must be computed by the user. In all cases these formulae were satisfied to better than eight significant figures. It is doubtful that any relevant errors were incurred here, as the other parameters are quoted to eight significant figures in Ref. 7. (ii) Twelve significant figures were retained in all matrix routines, so that no errors accumulated in the third significant figure of the results quoted here. (iii) The integrals were all calculated to a tolerance of 1 keV. This appears to be quite accurate, but there is a catch. All errors are incurred through the fact that one must sample the integrands over a finite integration grid. Consequently the error may be systematic rather than random.

The maximum possible effect of the integration errors can be estimated by *systematically* altering each integral by 1 keV in a direction such that one raised the eigenvalue. This produced nearly one-half an MeV repulsion. Consequently one is left with an upper bound of −24.1 MeV to be compared with the experimental value of −28.4 MeV. The rms radius was calculated to be 1.28 (10^{-13}) cm, in comparison with an experimental value of 1.44 (10^{-13}) cm.

The trial wave function contains a 5.36% admixture of the $^5D_0$ state. Since the Paris potential yields a 5.77% admixture of the $^3D_1$ state in ^{2}H, this result in the present calculation of ^{4}He is remarkably low. The reason can be found by carefully inspecting Table II. For the tensor interaction the three-body terms make a contribution of opposite sign to the two-body terms; and one sees consider-

TABLE III. Values of $K(i)$ for the α particle.

β	$K(^3S_1,\beta_i)$	$K(^1S_0,\beta_i)$	$K(T,\beta_i)$
0.1	−1.539	−1.852	−0.055
0.3	1.009	1.980	−1.002
0.5	1.182	0.517	3.855
0.7	1.538	2.500	3.701
0.9	5.017	2.953	−9.412

able cancellation at small values for β_i, which derive their strength from the long range components of the tensor interaction. This effect is obviously absent in ^{2}H, plays only a minor role in ^{3}H, but is very significant in ^{4}He due to the increasing number of three-body terms relative to the number of two-body terms. The short range part of the tensor interaction is significantly weakened in modern nuclear forces due to the effect of heavier vector mesons,[7,8] which makes the cancellation between two-body and three-body contributions at long range even more pronounced. Moreover, the three-body terms reinforce the two-body terms for the central components of the interaction. The resulting enhancement of the excited central terms further diminishes the importance of the tensor terms when channel coupling is taken into account. Recent considerations on nuclear saturation by Moszkowski[9] are dependent on a weakened tensor interaction, and there is no doubt that the cancellation in the long range components of the tensor force will play some role in saturation.

Normally one would require that the relative wave function for any two nucleons vanish as their separation approaches zero in a calculation with modern nuclear forces. In the present example, however, this condition has not been forcibly inserted. Rather it is left to the interaction operator to accomplish this through the calculation, and one can later test the derived wave function to see how well this condition is fulfilled. Let us define $\phi_{12}(0)$ to be the value of the unperturbed wave function at zero separation for the relative motion of two nucleons in a particular channel, and $\psi_{12}(0)$ to be its perturbed counterpart. The derived wave function yields

$$\left|\frac{\psi_{12}(0)}{\phi_{12}(0)}\right|^2 = 0.001 \quad (^1S_0 \text{ state})$$

$$= 0.016 \quad (^3S_1 \text{ state}) . \tag{29}$$

Calculations for the α particle have been previously reported; the most recent using the Reid[4,10–13] and Urbana[13] interactions. The most appropriate comparison is probably with the Urbana interaction, since this is a modern potential comparable to that of the Paris group. The energy eigenvalue for this case was -25.1 ± 0.4 MeV, neglecting Coulomb forces. It is amusing that not only the eigenvalue, but also the error, are quite comparable to the results in this section. The Urbana group also calculated ^{4}He using the Reid soft core potential, obtaining only -22.9 ± 0.5 MeV. This is consistent with the previous work with the Reid interactions; and it appears that one may conclude that the modern Paris and Urbana potentials yield binding energy for ^{4}He which is 2 or 3 MeV nearer the experimental value compared to the Reid potential.

V. CONCLUSION

The most obvious improvement one could make in the trial wave function is to refine the grid of values chosen for the β_i. It is possible to tell how far one should carry this refinement without completing the entire calculation. Since the components of the trial function are not all orthogonal one will eventually reach a grid so small that the elements of the matrices used in Eq. (11) may be obtained from each other by linear extrapolation; for example, one will have

$$E_2(\beta_n) = \tfrac{1}{2}[E_2(\beta_n+\Delta\beta)+E_2(\beta_n-\Delta\beta)] .$$

At this point one succeeds in producing singular matrices, and not in improving the eigenvalue. This fact can be helpful in guiding one to choose an improved grid.

Before refinement of the grid is warranted, however, there is another significant improvement that clearly must be investigated. The effective three-body terms in this calculation were found to be quite large, but there were no three-body correlations *specifically* built into the trial wave function. Consequently, it is doubtful that one has obtained the optimum contribution from the three- (and four-) body correlation energy.

In addition, investigations of the contribution of three-body nuclear forces (which are mediated through to the Δ isobar) to the binding energy of very light nuclei have recently been reported.[13,14] It appears that the contribution to the binding energy of the α particle could easily be in the range of 1—4 MeV.

It is a straightforward matter to incorporate both these improvements into the procedure developed in this paper. The difficulty involved in implementing the method will depend only on the new integrals encountered from the specific form of the nuclear three-body force.

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