

Two-Body Equations for Four-Nucleon Problems*

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(Received 24 October 1968)

The variational principle for the energy is used to derive integrodifferential equations for the two-body functions which, when combined in the product form, yield the "best" independent-pair wave function for the α particle. A practicable iteration procedure for finding approximate solutions to these equations is developed and is used to obtain an approximate ground-state wave function, for an example, four-body Hamiltonian for which the potential is central. Improvements in the iteration procedure are described which make it a feasible method for solving the integrodifferential equations even when tensor forces are included.

I. INTRODUCTION

FOLLOWING the ideas used by Delves and Derrick¹ and by Bodmer and Ali² to obtain the "best" pair wave functions for the three-body nuclei, we derive below the integrodifferential equations (IDE's) for the best pair wave function for the α particle. An exact iteration solution of these IDE's is not feasible in the four-body case, because the integrals in these equations are five-dimensional. To overcome this, an approximation is made so that these integrals can be reduced to one- and two-dimensional ones.

If, as assumed by Cohen,³ the α particle has total angular momentum 0, total isospin 0, and even parity, the ground state of the α particle can be written³ as the sum of 17 terms, each of which has a definite orbital angular momentum. By generalizing the procedure that is used in Sec. II and in the Appendix, one^{4,5} obtains 32 coupled IDE's for the 32 two-body functions which are to be combined to form the best independent-pair approximation for these 17 terms of the α -particle wave function.

The α -particle wave function consists of only the principal S state of Cohen's classification and the magnitudes of the other 16 terms are zero if the interaction between the nucleons is independent of spin and is central. In Sec. II, we derive a single IDE for the two-body function which is used to construct an independent-pair approximation for this S state. We solve this IDE in Sec. III for the example of a four-body Hamiltonian in which the interaction is given by the hard-core potential II of Ref. 6. After critically discussing this example in Sec. IV, we examine the feasibility of solving the set of two IDE's which are derived in the Appendix for the case in which tensor forces are included in the Hamiltonian and the prin-

cipal S and D states of Cohen's classification of the wave function are retained.

II. S-STATE EQUATION

A. Derivation of the IDE

If the interaction between the nucleons is assumed to be given by a spin-independent, central potential, the ground state of the α particle consists only of the principal S state of Cohen's classification and the magnitudes of the other 16 terms are zero. We write this S state as

$$\Psi_s = \Phi_s F_s(r_1, r_2, \dots, r_6), \quad (1)$$

with

$$\Phi_s = 2^{-1/2}(\varphi_1 \chi_2 - \varphi_2 \chi_1),$$

where r_1 to r_6 are the six interparticle distances illustrated in Fig. 1, the function F_s is symmetric in the interchange of any two of these six variables, and φ_1 and φ_2 , which are functions of the spin variables, and χ_1 and χ_2 , which are functions of the isospin variables, are defined by Cohen.³

In this section, we derive an IDE for a function $f_s(r)$ so that with the function F_s approximated by the product

$$F_s \approx \prod_{j=1}^6 f_s(r_j), \quad (2)$$

the upper bound to the ground-state energy as given by

$$E_u = (\Psi_s, H\Psi_s) / (\Psi_s, \Psi_s) \quad (3)$$

is the lowest possible for a wave function of this product form. The c.m. part of the wave function has been factored out and cancelled in these expressions.

The spin and isospin variables are easily summed out in Eq. (3), so that, using the functional form (2), we get

$$E_u = \left[\prod_{m=1}^6 f_s(r_m), \mathcal{H} \prod_{n=1}^6 f_s(r_n) \right] / \left[\prod_{m=1}^6 f_s(r_m), \prod_{n=1}^6 f_s(r_n) \right], \quad (4)$$

where

$$\mathcal{H} = \sum_{j=1}^6 T(r_j) + \sum_{(i,j,k)} S(r_i, r_j, r_k) + \sum_{j=1}^6 v(r_j), \quad (5)$$

* Work sponsored by the National Science Foundation.

¹ L. M. Delves and G. H. Derrick, *Ann. Phys. (N.Y.)* **23**, 133 (1963).

² A. R. Bodmer and Shamsher Ali, *Nucl. Phys.* **56**, 657 (1964).

³ L. Cohen, *Nucl. Phys.* **20**, 690 (1960); **22**, 492 (1961).

⁴ A derivation of this set of 32 equations is given by Van Dyke (Ref. 5). Actually, 34 equations are obtained, but two of these are not independent of the others.

⁵ P. Van Dyke, Ph.D. thesis, Lehigh University, 1968 (unpublished).

⁶ E. W. Schmid, Y. C. Tang, and R. C. Herndon, *Nucl. Phys.* **42**, 95 (1963).

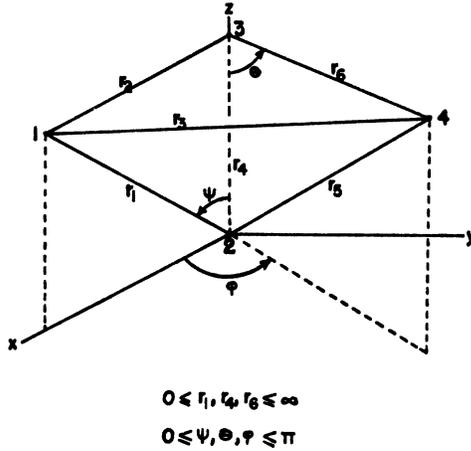


FIG. 1. Coordinates with nucleons at points marked 1-4.

in which the symbol (i, j, k) means that the sum is over all possible values of i, j , and k , so that r_i, r_j , and r_k form a triangle;

$$T(r_j) = -(\hbar^2/m)r_j^{-1}(\partial^2 r_j / \partial r_j^2),$$

$$S(r_i, r_j, r_k) = -(\hbar^2/2m)[(r_i^2 + r_j^2 - r_k^2)/r_j](\partial^2 / \partial r_i \partial r_j),$$

$v(r)$ is the central potential, and the scalar product $(,)$ is an integral over the six-dimensional space of the interparticle distances with the volume element and limits of integration that are given by Cohen and Willis.⁷

The variation of the functional form of the f_s to obtain the minimum of E_u leads to the condition

$$\int_0^\infty r_1 dr_1 \delta f_s(r_1) \left[\int d\tau_5 \left[\prod_{j=2}^6 f_s(r_j) \right] (\mathcal{H} - \lambda) \prod_{k=2}^6 f_s(r_k) \right] \times f_s(r_1) = 0, \quad (6)$$

where the integration over the variable r_1 is arbitrarily chosen to be written separately and integrated last. The total volume element $r_1 dr_1 d\tau_5$ and the limits of integration are chosen given by Cohen and Willis⁷ and mentioned above. In establishing Eq. (6), we use the Hermitian property of the operator \mathcal{H} and the symmetries of the Hamiltonian and wave function. The ground-state value of the Lagrange multiplier λ is equal to E_u .

Since the variation of the function f_s is arbitrary, we conclude that

$$\left[\int d\tau_5 \left[\prod_{j=2}^6 f_s(r_j) \right] (\mathcal{H} - \lambda) \prod_{k=2}^6 f_s(r_k) \right] f_s(r_1) = 0$$

⁷ L. Cohen and J. B. Willis, Nucl. Phys. **13**, 125 (1959).

or

$$-\frac{\hbar^2}{m} r_1^{-1} \frac{d^2(r_1 f_s(r_1))}{dr_1^2} + G(r_1) \frac{df_s(r_1)}{dr_1} + [v(r_1) + I(r_1)] f_s(r_1) = \lambda f_s(r_1), \quad (7)$$

where

$$I(r_1) = [B(r_1)]^{-1} \int d\tau_5 \left[\prod_{m=2}^6 f_s(r_m) \right] \times [4T(r_4) + T(r_6) + 2S(r_2, r_4, r_1) + 4S(r_6, r_2, r_3) + 2S(r_2, r_3, r_6) + 4v(r_4) + v(r_6)] \prod_{n=2}^6 f_s(r_n), \quad (8)$$

$$G(r_1) = -\frac{\hbar^2}{m} \frac{2}{B(r_1)} \int d\tau_5 \left[\prod_{m=2}^6 f_s(r_m) \right] \times \frac{r_1^2 + r_2^2 - r_4^2}{r_1 r_2} \frac{df_s(r_2)}{dr_2} \prod_{n=3}^6 f_s(r_n), \quad (9)$$

and

$$B(r_1) = \int d\tau_5 \prod_{m=2}^6 f_s^2(r_m). \quad (10)$$

B. Approximate Equation

It is not practicable to solve Eq. (7) exactly by iteration, because the integral terms, I , G , and B are five-dimensional integrals which require excessive computer time to evaluate by numerical integration. Instead, we choose to approximate these terms by replacing the functional form of $f_s(r)$ by

$$f_s(r) \approx N \exp(-\alpha r^2/2) \quad (11)$$

in those parts of the integrands which depend only on the average behavior of the function f_s and are not sensitive to the details of f_s . Thus, this substitution (11) is not made in the expressions $T(r)f_s(r)$ and $v(r)f_s(r)$.

As a result of this approximation, the lowest eigenvalue λ of Eq. (7) is no longer equal to E_u of Eq. (3). The criteria for choosing the parameter α are discussed as part of the example in Sec. III.

With the substitution of expression (11) as described above, the expressions (8)-(10) become

$$I(r_1) = [B(r_1)]^{-1} \int \{ 4 \exp(-\alpha R_4^2) f_s(r_4) [T(r_4) + v(r_4)] \times f_s(r_4) + \exp(-\alpha R_6^2) f_s(r_6) [T(r_6) + v(r_6)] f_s(r_6) - \frac{\alpha^2 \hbar^2}{m} \exp(-\alpha R^2) (4r_2^2 + r_6^2 - r_1^2) \} d\tau_5, \quad (12)$$

$$G(r_1) = -\frac{2\hbar^2}{mB(r_1)} \int \left(\exp(-\alpha R_4^2) f_s(r_4) \times \frac{r_1^2 + r_4^2 - r_2^2}{r_1 r_4} \frac{df_s(r_4)}{dr_4} \right) d\tau_5, \quad (13)$$

and

$$B(r_1) = \int \exp(-\alpha R^2) dr_6, \quad (14)$$

where

$$R^2 = \sum_{j=2}^6 r_j^2 \quad \text{and} \quad R_k^2 = R^2 - r_k^2.$$

The above integral expressions as written in the interparticle distance coordinates r_2 to r_6 are complicated by inseparabilities introduced by the volume element and the limits of integration as expressed in these coordinates. Cohen and Willis⁷ introduce new coordinates to remove these inseparabilities, but these are not convenient variables to use here because the interparticle distance which is labeled r_6 and is skew to the side labeled r_1 in Fig. 1 cannot be chosen as one of his coordinates. Thus, those integrals which contain operators in r_6 can not easily be evaluated. To overcome this, we introduce the coordinates $r_1, r_4, r_6, \psi, \theta,$ and φ as shown in Fig. 1, for which

$$r_2^2 = r_1^2 + r_4^2 - 2r_1 r_4 \cos\psi,$$

$$r_5^2 = r_4^2 + r_6^2 - 2r_4 r_6 \cos\theta,$$

and

$$r_3^2 = r_1^2 + r_4^2 + r_6^2 - 2r_4 r_6 \cos\theta - 2r_1 r_4 \cos\psi + 2r_1 r_6 (\cos\psi \cos\theta - \sin\psi \sin\theta \cos\varphi).$$

In these coordinates, the integrations involved in expressions (12)–(14) can be partially carried out. To illustrate this, consider Eq. (14) in these coordinates;

$$\begin{aligned} B(r_1) &= 16\pi^2 \exp(-2\alpha r_1^2) \int_0^\infty dr_4 r_4^2 \exp(-4\alpha r_4^2) \\ &\times \int_0^\infty dr_6 r_6^2 \exp(-3\alpha r_6^2) \int_0^\pi d\psi \sin\psi \int_0^\pi d\theta \sin\theta \\ &\times \int_0^\pi d\varphi \exp[4\alpha r_1 r_4 \cos\psi + 4\alpha r_4 r_6 \cos\theta \\ &+ 2\alpha r_1 r_6 (\sin\psi \sin\theta \cos\varphi - \cos\psi \cos\theta)]. \quad (15) \end{aligned}$$

We proceed by expanding the part of the last exponential factor which contains r_6 ,

$$\exp\{2\alpha r_6 [\cos\theta (2r_4 - r_1 \cos\psi) + r_1 \sin\psi \sin\theta \cos\varphi]\},$$

in a Taylor series in powers of its total argument. After the integration over φ is performed term by term, this series can be further expanded, by using the binomial expansion theorem, in powers of $r_1, r_4, r_6, \cos\psi,$ and $\cos\theta$. The resulting series is

$$\begin{aligned} \sum_{n=0}^{\infty} (2\alpha r_6)^n \sum_{m(\text{even})=0}^n \pi 2^{-m} \sum_{l=0}^{m/2} \sum_{k=0}^{m/2} \sum_{j=0}^{n-m} (-1)^{l+k+j} \\ \times \frac{r_1^{m+i} (2r_4)^{n-m-i} (\cos\psi)^{2l+i} (\cos\theta)^{2k+n-m}}{(\frac{1}{2}m-l)! l! (\frac{1}{2}m-k)! k! (n-m-j)! j!} \end{aligned}$$

Expression (15) is further manipulated by carrying out the elementary integrations over r_6 and θ to give

$$\begin{aligned} B(r_1) &= 4\pi^{7/2} (3\alpha)^{-3/2} \exp(-2\alpha r_1^2) \\ &\times \sum_{n(\text{even})=0}^{\infty} (\frac{1}{2}\alpha)^{n/2} \frac{(n+2)!}{(\frac{1}{2}n+1)!} \sum_{m(\text{even})=0}^n 2^{n-2m} \\ &\times \sum_{l=0}^{m/2} \frac{(-1)^l}{(\frac{1}{2}m-l)! l!} \sum_{k=0}^{m/2} \frac{(-1)^k}{(\frac{1}{2}m-k)! k! (2k+n-m+1)} \\ &\times \sum_{j=0}^{n-m} \frac{(-1)^{j+m+i}}{(n-m-j)! j! 2^j} J(n, m, l, j, \alpha, r_1), \end{aligned}$$

where

$$\begin{aligned} J(n, m, l, j, \alpha, r_1) &= r_1^{-(2l+i+1)} \int_{-r_1}^{r_1} dz z^{2l+i} \\ &\times \int_0^\infty dr_4 r_4^{n-m-j+2} \exp[-4\alpha(r_4^2 - zr_4)], \end{aligned}$$

in which the substitution $z = r_1 \cos\psi$ is used. The rates of convergence of this series for $B(r_1)$ and of the corresponding series that are obtained for $I(r_1)$ and $G(r_1)$ are rapid and independent of the values of the variable r_1 and parameter α . In all cases, the error is less than $\frac{1}{2}\%$ if the sum over n is cut off after seven terms.

There is one significant difference between the method of evaluating the integral expressions for $I(r)$ and $G(r)$ and that described above for $B(r)$. Since the approximate expression (11) cannot be used for $f_s(r_6)$ in part of the integrand of Eq. (12) for $I(r_1)$, the integration over r_6 in such terms must be performed numerically because $f_s(r_6)$ is specified only numerically from a numerical solution of Eq. (7) which is carried out in the previous cycle of an iteration procedure. Similarly, in some of the integrations over r_4 in Eqs. (12) and (13), the function $f_s(r_4)$ is taken to be this same numerical solution from the previous iteration cycle.

With this reduction of the integral expressions, an approximate solution of Eq. (7) for the function $f_s(r)$ can be obtained by the iteration procedure which was alluded to above. At each cycle of the iteration, the approximate forms for $G(r)$ and $I(r)$ are determined by the procedure just described, and then Eq. (7) is solved numerically for the function f_s that is used to determine $G(r)$ and $I(r)$ for the next cycle. Five such cycles are sufficient in the example reported in Sec. III.

III. AN EXAMPLE

As a test of this method, we use it to construct a product function of the form of Eq. (2) for the ground-state function of a four-body Hamiltonian in which the potential expression is given by $\frac{1}{2}$ the sum of the singlet and triplet parts of the hard-core potential II of Ref. 6.

The product function so obtained is used in Eq. (3) to calculate an upper bound to the ground-state energy

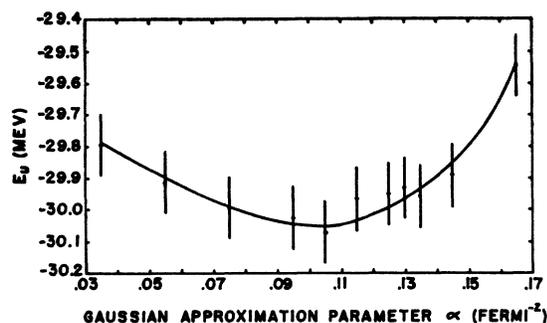


FIG. 2. Upper bound of the energy given by Eq. (3) for a range of the Gaussian parameter α . Vertical lines through points represent the possible range of values as estimated from the variance found in the Monte Carlo sampling.

for the Hamiltonian in which the Coulomb repulsion between the protons has been included. A Monte Carlo method of integration similar to that described by Herndon and Tang⁸ is used to evaluate the integrals in this expression. For 100 000 random samples, the uncertainty in the value of E_u obtained is less than 0.1 MeV as judged by the variance.

The wave function, and therefore the energy limit E_u that is obtained, depends on the parameter α that appears in the Gaussian approximation to the function f_s which is given by Eq. (11). This dependence of the energy is illustrated in Fig. 2. If we apply the usual variational-method criteria, the best value of α is that at the minimum of this curve: $\alpha = 0.105 \text{ F}^{-2}$. Since the minimum of the curve in Fig. 2 is so broad, it is clear that the value of α is not critical. We give the reasons for this in Sec. IV.

Fortunately, it is not necessary to calculate the values of E_u for a range of α as was done in this example for illustrating the method. A value of α near that at the minimum of the curve in Fig. 2 is given as the solution

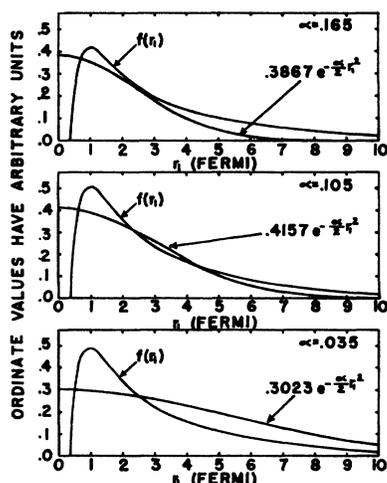


FIG. 3. Two-body function $f(r)$ and its Gaussian approximation for three values of α .

⁸ R. C. Herndon and Y. C. Tang, in *Methods in Computational Physics*, edited by B. Alder *et al.* (Academic Press Inc., New York, 1966), p. 153.

to the condition that the rms radii obtained for the function $f_s(r)$ and its Gaussian approximation in Eq. (11) be equal. This condition can be made part of the iteration process that is used to solve for f_s , and so the computer time to solve the entire problem is reduced to the time that is used to obtain any one point shown in Fig. 2. That this criterion yields a value for α close to the value at the minimum of the E_u -versus- α curve is demonstrated by the curves given in Fig. 3, in which the function f_s and the corresponding Gaussian function are compared for three values of the parameter α .

The errors in the evaluation of the coefficients $G(r)$ and $I(r)$ in Eq. (7) which are due to the replacement of the Gaussian function for $f_s(r)$ increase as r becomes large. Fortunately, the correct asymptotic behavior of $f_s(r)$ is known⁹ to be

$$f_s(r) \sim r^{-1/3} \exp\{-[(m/6\hbar^2)(B_4 - B_3)]^{1/2} r\}, \quad (16)$$

where B_3 and B_4 are the binding energies of the three-

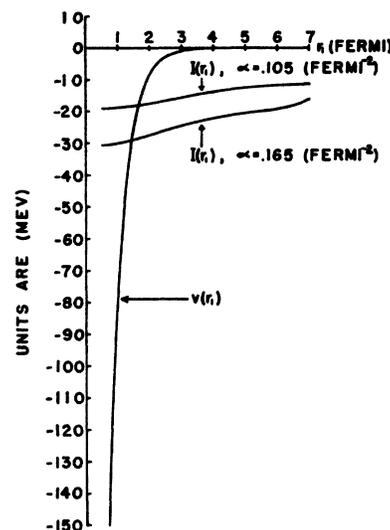


FIG. 4. Nonlocal potential $I(r_1)$ for two values of the Gaussian parameter α . For comparison, the local potential $v(r_1)$ is shown.

and four-body systems, respectively, with the same interaction between the nucleons. Sufficiently accurate values of B_3 and B_4 can be obtained by the procedure described by Mang and Wild.¹⁰

In the example reported here, we use expression (16) for $r > 7 \text{ F}$ and use Eq. (7) to continue the function for smaller values of r .

IV. DISCUSSION

A. Comparison with Other Methods

The example discussed in Sec. III was selected because other calculated values for the binding energy of the four-body system with this same interaction are

⁹ The asymptotic behavior of the α -particle wave function is, of course, very complicated. This simple behavior (Ref. 11) is correct only within the limits of the validity of the independent-pair approximation. A complete discussion of this for the three-body systems is given by Bodmer and Ali (Ref. 2).

¹⁰ H. J. Mang and W. Wild, *Z. Physik* **154**, 182 (1959).

available^{6,11} for comparison. We get (with the Coulomb repulsion between the protons included in the Hamiltonian)

$$E_u = -30.07 \pm 0.10 \text{ MeV},$$

while one of us obtains¹¹

$$E_u = -30.39 \pm 0.15 \text{ MeV}$$

by another method.

If, as described in Sec. III, the parameter α is determined to give a consistent rms radius as part of the iteration procedure that is used to get an approximate solution to Eq. (7), it takes about 2 min on a CDC 6600 computer to carry out five cycles of this iteration. While this is slightly longer than was used to solve the same example by the method described in Ref. 11, it is not yet clear which of these methods is better when noncentral forces are included in the Hamiltonian.

B. Future Improvements

As noted in Sec. III, the wave function and the energy E_u that are obtained do not depend sensitively on the value of the parameter α which appears in the expressions that are used to approximate the coefficients $I(\mathbf{r})$ and $G(\mathbf{r})$ in Eq. (7). The reason for this insensitivity is that the nonlocal terms $G(\mathbf{r})$ and $I(\mathbf{r})$ are small, smooth, slowly varying functions of \mathbf{r} which have only a small effect compared to other operators in Eq. (7) such as the potential $v(\mathbf{r})$. This condition is particularly true for $I(\mathbf{r})$, which is nearly constant, as illustrated in Fig. 4, and therefore the effect of this nonlocal potential is to contribute to the eigenvalue λ without significantly affecting the wave function. Thus, even though these nonlocal potentials change as α is varied (see Fig. 4), the solution for $f_s(\mathbf{r})$ does not change much.

Because the solution is not sensitively dependent on the terms $I(\mathbf{r})$ and $G(\mathbf{r})$ and these terms are smooth functions anyway, one is justified in replacing $I(\mathbf{r})$ and $G(\mathbf{r})$ by simple analytic functions which are adjusted to be equal to the values calculated for $I(\mathbf{r})$ and $G(\mathbf{r})$ at a few values of \mathbf{r} . This replacement reduces the computer time significantly so that one can realistically attempt to solve the two coupled IDE's (A3) and (A4) for the two pair wave functions which are to be used to form the best independent-pair approximation to the dominant S and D states of the α -particle wave function. Even with this simplification, we estimate the time needed to solve these coupled IDE's to be about 20 times that used to solve the single equation for the S state alone. We plan to carry out such a calculation soon.

APPENDIX

In this Appendix, the potential between each pair of particles is assumed to be of the form

$$V(j, k) = \left[\frac{1}{2}(1 + P_{jk}^\sigma) V_3(\mathbf{r}_{jk}) + \frac{1}{2}(1 - P_{jk}^\sigma) V_1(\mathbf{r}_{jk}) + S_{jk} V_T(\mathbf{r}_{jk}) \right] \left[\frac{1}{2}(1 + P_{jk}^\tau) \right],$$

¹¹ R. Folk, Nucl. Phys. A122, 353 (1968).

where \mathbf{r}_{jk} is the distance between particles j and k , and P_{jk}^σ and P_{jk}^τ are the spin- and space-exchange operators, respectively. The terms $V_3(\mathbf{r}_{jk})$ and $V_1(\mathbf{r}_{jk})$ are the triplet- and singlet-central even potentials and the term $S_{jk} V_T(\mathbf{r}_{jk})$ is the tensor-even potential, where

$$S_{jk} = 3(\boldsymbol{\sigma}_j \cdot \mathbf{r}_{jk})(\boldsymbol{\sigma}_k \cdot \mathbf{r}_{jk}) / r_{jk}^2 - \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_k.$$

We may retain here only the spatially symmetric S and D states of Cohen's classification,⁸ since, as others¹² have argued, the magnitudes of the other 15 states are small. The structure of the space-symmetric S state is given in Eq. (1) and that of the space-symmetric D state is

$$\Psi_D = \Phi_D F_D(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_6), \quad (\text{A1})$$

where

$$\Phi_D = (2)^{-1/2} \{ \varphi_D([22], ss) \chi_1 - \varphi_D([22], aa) \chi_2 \},$$

$$\varphi_D([22], aa) = D(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2),$$

$$\varphi_D([22], ss) = (3)^{-1/2} (D(\mathbf{r}, \mathbf{r}) - \frac{1}{2} D(\boldsymbol{\rho}_1, \boldsymbol{\rho}_1) - \frac{1}{2} D(\boldsymbol{\rho}_2, \boldsymbol{\rho}_2))$$

$$D(\mathbf{a}, \mathbf{b}) = [(\boldsymbol{\sigma}_1 \cdot \mathbf{a})(\boldsymbol{\sigma}_3 \cdot \mathbf{b}) + (\boldsymbol{\sigma}_3 \cdot \mathbf{a})(\boldsymbol{\sigma}_1 \cdot \mathbf{b}) - \frac{2}{3}(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_3)(\mathbf{a} \cdot \mathbf{b})] \varphi_1,$$

$$\mathbf{r} = \frac{1}{2}(\mathbf{r}_2 + \mathbf{r}_6), \quad \boldsymbol{\rho}_1 = 2^{-1/2} \mathbf{r}_1, \quad \boldsymbol{\rho}_2 = 2^{-1/2} \mathbf{r}_6,$$

and where the spin function φ_1 and the isospin functions χ_1 and χ_2 are defined by Cohen.⁸ The function F_D , which is symmetric, is approximated by the product form

$$F_D \approx \prod_{j=1}^6 f_D(\mathbf{r}_j), \quad (\text{A2})$$

which is the same structure as is given for F_s by Eq. (2).

In this case the requirement $\delta E_u = 0$ for arbitrary $\delta f_s(\mathbf{r}_1)$ and $\delta f_D(\mathbf{r}_1)$ yields a pair of coupled IDE's

$$L_{SS}(\mathbf{r}_1) f_s(\mathbf{r}_1) + L_{SD}(\mathbf{r}_1) f_D(\mathbf{r}_1) = 0 \quad (\text{A3})$$

and

$$L_{DD}(\mathbf{r}_1) f_D(\mathbf{r}_1) + L_{SD}(\mathbf{r}_1) f_s(\mathbf{r}_1) = 0, \quad (\text{A4})$$

where

$$L_{SS}(\mathbf{r}_1) = \int d\tau_6 \left[\prod_{j=2}^6 f_s(\mathbf{r}_j) \right] \langle \Phi_s | H - \lambda | \Phi_s \rangle \prod_{k=2}^6 f_s(\mathbf{r}_k),$$

$$L_{SD}(\mathbf{r}_1) = \int d\tau_6 \left[\prod_{j=2}^6 f_s(\mathbf{r}_j) \right] \langle \Phi_s | H - \lambda | \Phi_D \rangle \prod_{k=2}^6 f_D(\mathbf{r}_k),$$

and

$$L_{DD}(\mathbf{r}_1) = \int d\tau_6 \left[\prod_{j=2}^6 f_D(\mathbf{r}_j) \right] \langle \Phi_D | H - \lambda | \Phi_D \rangle \prod_{k=2}^6 f_D(\mathbf{r}_k).$$

The scalar product $\langle \rangle$ is a sum over the spin and isospin coordinates.

¹² G. Abraham, L. Cohen, and A. S. Roberts, Proc. Phys. Soc. (London) 68, 265 (1955).

It is interesting and important that, as pointed out by Cohen,³ the expressions obtained by this sum over the spin and isospin coordinates depend only on the interparticle distances r_1 to r_6 . In particular, these expressions do not depend on the Euler angles which can be used to give the orientation of the tetrahedron that is defined by these six interparticle distances. Thus we are spared the horrendous task of converting the kinetic energy operator to the interparticle distances and Euler angle coordinates as is done by Derrick¹³ for the easier three-body problem. Nevertheless, the spin sums lead to a very long expression for the kinetic energy part of L_{DD} .

A technique for simplifying the spin sum procedure is described by Irving¹⁴ and by Van Dyke.⁵ For L_{SS} we get

$$L_{SS}(r_1) = \int d\tau_6 \left[\prod_{j=2}^6 f_s(r_j) \right] (\mathcal{K} - \lambda) \prod_{k=2}^6 f_s(r_k), \quad (\text{A5})$$

where, in expression (5) for the operator \mathcal{K} , we substitute $v(r) = \frac{1}{2}[V_1(r) + V_3(r)]$.

With the spin sums carried out, the operator L_{SD} is

$$\begin{aligned} L_{SD}(r_1) = & -\frac{1}{2}r_1^{-2}V_T(r_1) \int d\tau_6 \left[\prod_{j=2}^6 f_s(r_j) f_D(r_j) \right] \\ & \times \left[-\frac{1}{3}r_1^2(r_1^2 + 4r_2^2 - 2r_6^2) + 2r_8^2(r_2^2 - r_4^2) \right] - 2 \int d\tau_6 \\ & \times \left[\prod_{j=2}^6 f_s(r_j) f_D(r_j) \right] \{ r_4^{-2}V_T(r_4) \left[-\frac{1}{3}r_4^2(r_1^2 + r_2^2 + r_4^2 \right. \\ & \left. + r_6^2 + r_6^2 - 2r_8^2) + r_2^2r_6^2 + r_1^2r_6^2 - r_2^2r_6^2 - r_1^2r_6^2 \right] \\ & \left. + \frac{1}{2}r_6^{-2}V_T(r_6) \left[-\frac{1}{3}r_6^2(r_6^2 + 4r_2^2 - 2r_1^2) + 2r_4^2(r_2^2 - r_8^2) \right] \right\}. \end{aligned} \quad (\text{A6})$$

After the spin sums are performed, the expression

obtained for L_{DD} becomes very long, and, since it is given in Ref. 5, we do not give it here.

By rearranging the various terms in L_{SS} and L_{DD} , we can write Eqs. (A3) and (A4) in the form

$$\begin{aligned} & -\frac{\hbar^2}{m} r_1^{-1} \frac{d^2(r_1 f_s(r_1))}{dr_1^2} + G(r_1) \frac{df_s(r_1)}{dr_1} \\ & + [v(r_1) + I(r_1)] f_s(r_1) + \frac{L_{SD}(r_1)}{B(r_1)} f_D(r_1) = \lambda f_s(r_1) \end{aligned} \quad (\text{A7})$$

and

$$\begin{aligned} & -\frac{\hbar^2}{m} r_1^{-1} \frac{d^2(r_1 f_D(r_1))}{dr_1^2} + K(r_1) \frac{df_D(r_1)}{dr_1} + M(r_1) f_D(r_1) \\ & + \frac{L_{SD}(r_1)}{C(r_1)} f_s(r_1) = \lambda f_D(r_1), \end{aligned} \quad (\text{A8})$$

where $G(r_1)$, $I(r_1)$, $B(r_1)$, and $L_{SD}(r_1)$ are given, respectively, by Eqs. (8), (9), (10), and (A6), and

$$C(r_1) = \int d\tau_6 \prod_{m=2}^6 f_D^2(r_m).$$

The terms $K(r_1)$ and $M(r_1)$ are integral expressions which are the parts of the operator $L_{DD}(r_1)$, which is given in Ref. 5, that are not given explicitly in Eq. (A8).

The iteration solution of the two coupled IDE's (A7) and (A8) for the pair functions $f_s(r_1)$ and $f_D(r_1)$ proceeds in a manner similar to that described for solving Eq. (7). A second Gaussian approximation in addition to that given by Eq. (11) for $f_s(r)$ is used for $f_D(r)$, i.e., $f_D(r) \approx N_D e^{-\beta r^2/2}$. The Gaussian parameters can be efficiently determined by the conditions that the functions have the same rms radii as their corresponding Gaussian approximation.

By incorporating the time-saving techniques which are discussed in Sec. IV B, this iteration procedure for obtaining f_s and f_D becomes a practicable method.

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