

Energy Levels of He^5 and Li^5 †

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The energies of the first three levels in He^5 are determined using a variational procedure. The various wave functions adopted incorporate alpha, triton, and deuteron correlations. It is determined that the ground state ($\frac{3}{2}-$) must be an alpha-neutron configuration whereas the ($\frac{1}{2}-$) level, which must also be described by this configuration, is not a sharp resonant state. The ($\frac{3}{2}+$) level at 16.69 Mev is shown to be a deuteron-triton configuration. The resultant energies and structures of these levels are in accord with the experimental situation. It should be stressed that our wave functions differ appreciably from the standard shell-model ones in the intermediate-coupling picture.

I. INTRODUCTION

THIS will be the second in a series of papers devoted to the low-lying energy levels of the light nucleus. In a previous paper¹ (hereafter referred to as I), we examined the behavior of the first few levels in Be^8 and Li^7 on the basis of the cluster model² in which a long-range correlation factor is introduced. These correlations manifest themselves as preferred clustering in nuclei. By choosing the appropriate cluster wave function, one can then determine a reasonably good upper bound to the binding energies of the various levels by the standard Ritz variational procedure.

This present work was motivated by a speculation presented in I, wherein we contended that the first "change-of-parity level" in Li^7 most probably will arise from a cluster structure substantially different from that of the ground state, namely, one in which the triton cluster is fractured. In our picture, a similar situation should prevail for the ($\frac{3}{2}+$) level in He^5 .³ This state, rather than being characterized by an alpha cluster and a neutron in some mode of relative motion, would be described by a triton cluster and a deuteron cluster in a relative s state. The presence of such a configuration would account for the well-known resonance in the deuteron-triton collision. Moreover, such a picture would explain why this excited level had an assignment of ($\frac{3}{2}+$) rather than the ($\frac{1}{2}+$) assignment which an alpha cluster plus neutron wave function would predict or the ($\frac{5}{2}+$) result one would expect from a standard shell model prediction. In addition, the fact that the reduced width approaches the Wigner limit⁴ strongly indicates the deuteron-triton configuration.⁵

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¹ L. D. Pearlstein, Y. C. Tang, and K. Wildermuth, *Nuclear Phys.* (to be published); see also *Bull. Am. Phys. Soc.* **4**, 271 (1960).

² K. Wildermuth and Th. Kanellopoulos, *Nuclear Phys.* **1**, 150 (1958); **9**, 449 (1958/59); CERN Report 59-23 (unpublished). We remark here that the ideas of the cluster model are basically similar to those of the resonating group method devised by J. A. Wheeler [*Phys. Rev.* **52**, 1083, 1107 (1937)].

³ F. Aijzenberg and T. Lauritsen, *Nuclear Phys.* **11**, 1 (1959).

⁴ L. Eisenbud and E. P. Wigner, *Nuclear Structure* (Princeton University Press, Princeton, New Jersey, 1958).

⁵ W. E. Kunz, *Phys. Rev.* **97**, 456 (1955).

To continue the systematic examination of the light nucleus, we have also conducted a detailed analysis of the ground state and possible first excited state of He^5 . The relevant cluster structure would now be an alpha cluster plus nucleon in a relative p state, with the two-body spin-orbit potential accounting for the splitting. The presence or absence of a relative minimum in the total energy as a function of the variational parameters would then be the determining factor for the occurrence of a resonant state.

In the next section, the method of calculation as applied to the low-lying negative parity levels is described. Section III is devoted to the ($\frac{3}{2}+$) level at 16.69 Mev. The remaining section (Sec. IV) contains a review of our results and a discussion of all conclusions.

II. GROUND STATE OF He^5

The procedure for evaluating the energy of a given level has been thoroughly discussed in I; consequently we shall present only a brief review of the method at this time. Since we are presently concerned with the ($\frac{3}{2}-$) and ($\frac{1}{2}-$) states, we shall limit ourselves to a description of the calculation as applied to these states. The appropriate cluster wave function would then have the symbolic form

$$\Psi = A \Phi_0(\alpha) \chi(\mathbf{R}_\alpha - \mathbf{R}_n), \quad (1)$$

in which $\Phi_0(\alpha)$ refers to a wave function which describes an alpha cluster and $\chi(\mathbf{R}_\alpha - \mathbf{R}_n)$ pertains to the relative motion between the neutron and the alpha cluster. The operator A signifies the complete antisymmetrization of the wave function with respect to all pairs of particles.

The quantity of ultimate interest would be the expectation value of the Hamiltonian. For this study, we choose the standard form for this operator given by

$$H = - \frac{\hbar^2}{2M} \sum_{\text{all particles}} \nabla_i^2 + \sum_{\text{all pairs}} V_{ij}, \quad (2)$$

where V_{ij} is the two-body potential. The procedure for computing with this Hamiltonian is now described. Assuming that a hard-core force is important only for the mutual interaction of the particles within a cluster,¹

we determine the interaction of the outside nucleon with the alpha cluster by employing a Serber force of nonsaturating character, but one which is in accord with all low-energy two-nucleon phenomena. Once this energy, which shall hereafter be referred to as the "interaction energy," has been computed, there remains only the necessity of determining the binding energy of the alpha cluster. Recently, this calculation has been performed by Mang and Wild,⁶ in which the results are presented as a relationship between the binding energy of the alpha cluster and the width parameter which determines the size of this cluster. (The limitations of this relationship will be discussed in the next section.) The procedure then, is to compute the expectation value of the Serber potential; discard that part of the energy which pertains to the internal energy of the alpha cluster, the remainder being the interaction energy; add the correct value for the alpha cluster internal energy as determined by the aforementioned authors; and minimize with respect to all variational parameters, the result being the energy of the appropriate level in He⁶ and Li⁶.⁷

To proceed, we choose for our trial wave function

$$\Psi = A\psi(1234; 5) \\ = A \left\{ \exp\left(-\frac{\alpha}{2} \sum_{i=1}^4 r_{iD}^2\right) R^n \exp(-\frac{2}{3}\beta R^2) Y_{lm}(\mathbf{R}/R) \right\}, \quad (3)$$

with $n=l=1$. In Eq. (3),

$$\mathbf{r}_{iD} = \mathbf{r}_i - \mathbf{R}_\alpha, \quad (4)$$

and

$$\mathbf{R} = \mathbf{R}_\alpha - \mathbf{R}_n, \quad (5)$$

with

$$\mathbf{R}_\alpha = \frac{1}{4} \sum_{i=1}^4 \mathbf{r}_i. \quad (6)$$

Also note that in Eq. (3), we have for brevity suppressed the spin and isobaric spin coordinates.

The appropriate Serber potential⁸ has the form

$$V_{ij} = -V_0 \exp(-\kappa r_{ij}^2) \{w(1 + P_{ij}^s) + b(P_{ij}^{s\sigma} - P_{ij}^{\tau})\} \\ - V_{LS} \exp(-\lambda r_{ij}^2) (\mathbf{r}_i - \mathbf{r}_j) \times (\mathbf{p}_i - \mathbf{p}_j) \\ \cdot (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j) \hbar^{-1}/2, \quad (7)$$

wherein $V_0 = 68.6$ Mev, $\kappa = 4.16 \times 10^{25}$ cm⁻², $w = 0.41$, $b = 0.09$, and P_{ij}^s , $P_{ij}^{s\sigma}$, P_{ij}^{τ} represent the space, spin, and isobaric spin exchange operators, respectively. Also, in Eq. (7), $\boldsymbol{\sigma}_i$ is the Pauli spin operator. The range (λ) and depth (V_{LS}) of the spin-orbit potential

⁶ H. J. Mang and W. Wild, Z. Physik **154**, 182 (1959).

⁷ In the case of Li⁶, we must add the appropriate interaction Coulomb energy.

⁸ Lederer, *Diplomararbeit* (München, 1957, unpublished).

will be discussed when the results of our calculation are presented. Our particular choice for the wave function is dictated by our desire to have it coincide with the shell model one when α is equal to β . The fact that, in general, α is not equal to β indicates the presence of highly excited shell-model states in our particular wave function.

A. The Normalization, Kinetic and Potential Integrals

We now present the complete expression for the expectation value of the Hamiltonian operator. For reasons of brevity, the detailed form of the results and methods of calculation will be exhibited in Appendix I; here, we only present the general form of the various contributions. The normalization factor is easily seen to be

$$N^2 = 5! \int (\psi_0 - \psi_1)^* \psi_0 d\tau, \quad (8)$$

in which

$$\psi_0 = \psi(1234; 5), \quad \psi_1 = \psi(5234; 1). \quad (9)$$

The definitions of Eq. (9) are self-evident and are equivalent to those used by several authors.⁹ The important point to note is that the first four slots in the wave function are saturated in the spin and isobaric spin coordinates; consequently, the filling of those four positions describes an alpha cluster. Moreover, we see that there is only one possible exchange which contributes (ψ_1), a direct consequence of orthogonality due to the particular choice of this spin and isobaric spin dependence of ψ_0 . The factor $5!$ appearing in Eq. (9) accounts for the total number of permutations of the individual nucleons.

Next, the expectation value of the kinetic energy operator, $-(\hbar^2/2M) \sum_i \nabla_i^2$, can be written in the form¹⁰

$$\langle T \rangle = (\hbar^2/2M) (2n\beta + 3\beta + 9\alpha) \\ - 5! \frac{\hbar^2}{2M N^2} \int (\psi_0 - \psi_1)^* \left(-2\alpha^2 \frac{\partial}{\partial \alpha} - 2\beta^2 \frac{\partial}{\partial \beta} \right) \psi_0 d\tau \\ - 5! \frac{\hbar^2}{2M} \frac{n(n+1) - l(l+1)}{0.8N^2} \int (\psi_0 - \psi_1)^* \frac{1}{R^2} \psi_0 d\tau. \quad (10)$$

For the present case, we set $n=l=1$. For a later analysis we shall make other choices.

Finally, the expectation value of the potential energy operator is computed and, after some algebraic

⁹ See, for example, S. F. Edwards, Proc. Cambridge Phil. Soc. **48**, 652 (1952).

¹⁰ The center-of-mass motion of the nucleus can be easily split off in our cluster wave function. This has the consequence that in our calculations, we need not worry about the excitation of spurious states.

manipulation, can be cast in the form

$$\begin{aligned}
 \langle V \rangle &= \langle V_G \rangle + \langle V_{SO} \rangle \\
 &= (5!/N^2) \left\{ \int \psi_0^* [w(12F_{12} + 3F_{16})] \psi_0 d\tau \right. \\
 &\quad \left. - \int \psi_1^* [w(12F_{12} + 6F_{23} - 3F_{16})] \psi_0 d\tau \right\} \\
 &\quad + (5!/N^2) \left\{ \int \psi_0^* (2G_{15}) \psi_0 d\tau \right. \\
 &\quad \left. - \int \psi_1^* (G_{15} + G_{25}) \psi_0 d\tau \right\} \Gamma, \quad (11)
 \end{aligned}$$

wherein

$$F_{ij} = -V_0 \exp(-\kappa r_{ij}^2) \quad (12)$$

and G_{ij} is the z -component of the space part of the two-body spin-orbit force of the neutral form given by¹¹

$$G_{ij} = -[V_{LS} \exp(-\lambda r_{ij}^2) (\mathbf{r}_i - \mathbf{r}_j) (\mathbf{p}_i - \mathbf{p}_j)]_z \hbar^{-1}. \quad (13)$$

In Eq. (11), Γ is equal to 1 (−2) for the $\frac{3}{2}$ ($\frac{1}{2}$) state. For this particular cluster configuration, the expectation value of the spin and isobaric spin exchange potentials (Bartlett and Heisenberg forces) have exactly the same values and consequently, do not contribute. It should further be remarked that the spin-orbit potential only acts between pairs of particles having the same z component of spin.

B. Numerical Analysis

The previous considerations lead to an expression for the expectation value of the Hamiltonian in terms of the variational parameters, α and β . Setting $\beta=0$ in the aforementioned expression and subtracting that result from the general expression for the energy determines the interaction energy. Finally, by adding the Mang and Wild result for the internal energy of the alpha cluster, we obtain the energy of the state in question, which must now be minimized with respect to α and β . Since the result for the internal energy of the alpha cluster was in graphical form, it has been fit by the analytic expression given by

$$E_\alpha = -28.3 + 33.4(1 - 0.96/y)^2 \text{ Mev}, \quad (14)$$

where for computational purposes, we have redefined the variational parameters as

$$x = \beta/\alpha, \quad y = \kappa/\alpha. \quad (15)$$

We like to point out here that, actually, Mang and Wild did a self-consistent calculation only for the binding energy of the free alpha particle; hence, strictly speaking, one cannot extract the compressibility of an alpha particle from their results.¹² Nevertheless, it is still possible to employ the above equation for E_α in

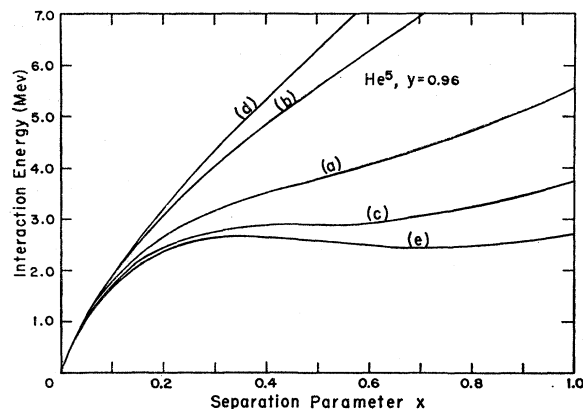


FIG. 1. Interaction energy as a function of the separation parameter for the $\frac{3}{2}$ (—) and $\frac{1}{2}$ (—) states in He^5 : (a) spin-orbit interaction not included, i.e., $V_{LS}=0$; (b) $\frac{1}{2}$ (—) state with $V_{LS}=4.5$ Mev and $\lambda=2.657 \times 10^{25} \text{ cm}^{-2}$; (c) $\frac{3}{2}$ (—) state with $V_{LS}=4.5$ Mev and $\lambda=2.657 \times 10^{25} \text{ cm}^{-2}$; (d) $\frac{1}{2}$ (—) state with $V_{LS}=13.8$ Mev and $\lambda=4.16 \times 10^{25} \text{ cm}^{-2}$; (e) $\frac{3}{2}$ (—) state with $V_{LS}=13.8$ Mev and $\lambda=4.16 \times 10^{25} \text{ cm}^{-2}$.

our computation for the following reasons: (1) the alpha cluster in our particular case is not very different in size from a free alpha particle; (2) our result is rather insensitive to the compressibility of the alpha particle; and (3) the compressibility corresponding to the Mang and Wild calculation is quite consistent with the nuclear compressibility determined from analyses of the isotope shifts.¹³ We further remark here that the analytic fit given by Eq. (14) does not actually correspond to the form quoted by the aforementioned authors. Rather, their curve has been translated with the shape unaltered to arrive at the correct alpha particle rms radius and binding energy.

The complete numerical analysis was performed on an IBM-650 computer. A selective set of results for the interaction energy are depicted in Fig. 1 in the form of a graph in which this energy is plotted as a function of x with y at its optimizing value¹⁴ of 0.96. This value corresponds very closely to the free alpha particle width parameter. We note [see curve (a)] that without the spin-orbit potential, there is no actual minimum for either state. However, the introduction of such an interaction can produce a relative minimum for the $\frac{3}{2}$ (—) state since the force is attractive in this state. Conversely, we conclude that under no circumstances can there be a narrow resonant ($\frac{1}{2}$ —) level in He^5 , a result which is consistent with experiment, since it has been established that the appropriate scattering phase shift does not pass through 90° .¹⁵

Since there has been no complete systematic examination of a spin orbit interaction in the low-energy two-nucleon phenomena, we must resort to inferences

¹³ D. L. Hill, *Encyclopedia of Physics* (Springer-Verlag, Berlin, 1957), Vol. 39, p. 203.

¹⁴ By optimizing value of y , we mean that value which yields the minimum energy of the state in the variational procedure.

¹⁵ K. W. Brockman, *Phys. Rev.* **108**, 1000 (1957).

¹¹ J. P. Elliott and A. M. Lane, *Phys. Rev.* **96**, 1160 (1954).

¹² We thank Dr. W. Brenig for pointing this out to us.

made from considerations of more complex systems. Such an examination has been performed by Hochberg et al.¹⁶ in which they infer the range and depth of the spin-orbit potential by considering nucleon-alpha scattering. Consequently, we have performed our analysis using these values and obtained the results represented by curves (b) and (c) in Fig. 1. Also, we have examined the case in which the range of the spin-orbit potential is equal to that of the central potential. The depth is then determined from a relationship between range and depth formulated by Blin-Stoyle.¹⁷ The ensuing interaction energy is depicted by curves (d) and (e). It should be remarked at this point that this latter relationship was derived on the basis of two assumptions: (1) Antisymmetrization of the outside nucleon with the central core is unimportant, a result which is approximately borne out by our calculation, and (2), the spin-orbit force is short-ranged, i.e., $\lambda \gg \alpha$, a situation which is violated by the present choice of range. Thus the depth of the potential is overestimated. The total energies resulting from the above two choices are listed along with the experimental value in Table I.

III. EXCITED STATE OF He^5

As we have previously discussed, we would expect that the $(\frac{3}{2}^+)$ level at 16.69 Mev in He^5 is primarily a deuteron-triton configuration.¹⁸ However, for the sake of consistency, we must show that the alpha-neutron configuration in relative s and d states cannot properly describe resonant states. Consequently, we have performed the desired calculation including the central potential only and determined the interaction energy which is plotted in Fig. 2 as a function of x with y chosen to give the free alpha particle radius. The form of those curves is completely insensitive to the value of y . We note that these curves possess no relative minima¹⁹ and therefore, we conclude that the $(\frac{3}{2}^+)$

TABLE I. Energy of $(\frac{3}{2}^-)$ state in He^5 .

Constants in the spin-orbit potential	x	y	E_{cal} (Mev)
$V_{LS} = 4.5 \text{ Mev}^a$ $\lambda = 2.657 \times 10^{25} \text{ cm}^{-2}$	0.52	0.96	-25.4
$V_{LS} = 13.8 \text{ Mev}$ $\lambda = 4.16 \times 10^{25} \text{ cm}^{-2}$	0.75	0.96	-25.9
$E_{\text{exp}} = -27.3 \text{ Mev}$			

^a Taken from Hochberg et al., reference 16.

¹⁶ S. Hochberg, H. S. W. Massey, H. Robertson, and L. H. Underhill, Proc. Phys. Soc. (London) **A68**, 746 (1955).

¹⁷ R. J. Blin-Stoyle, Phil. Mag. **46**, 973 (1955).

¹⁸ Due to the nature of the two-body force which we use, the $(\frac{3}{2}^+)$ state resulting from such a configuration will have a higher excitation energy.

¹⁹ When the alpha cluster and the neutron is in a relative d -state motion, spin-orbit interaction should also be included. It is obvious, however, that no reasonable spin-orbit force can possibly produce a relative minimum.

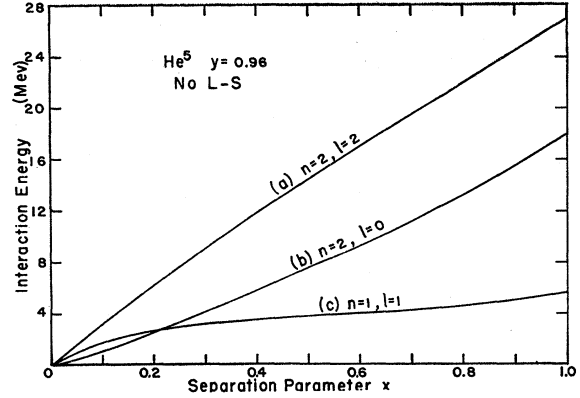


FIG. 2. Interaction energy as a function of the separation parameter for the alpha-nucleon configuration with the choices: (a) $n=2, l=2$, (b) $n=2, l=0$, and (c) $n=1, l=1$.

state contains, at first, no contribution from the alpha-nucleon configuration. The rate at which this state forms the unstable configuration determines the partial width for the alpha-neutron decay. A rough estimation indicates that this process is rather slow compared to the decay into a deuteron and a triton. Consequently, we choose

$$\Psi = A \Phi_0(TR) \Phi_0(D) \chi(\mathbf{R}_{TR} - \mathbf{R}_D) \quad (16)$$

to represent the state in question. The various constituents of the wave function are defined by

$$\Phi_0(TR) = \exp \left\{ -\frac{\alpha}{2} \sum_{i=1}^3 r_{iD}^2 \right\}, \quad (17)$$

$$\Phi_0(D) = \exp \left\{ -\frac{\bar{\alpha}}{2} \sum_{j=5}^6 r_{jD}^2 \right\},$$

$$\chi(\mathbf{R}_{TR} - \mathbf{R}_D) = R^n Y_{lm}(\mathbf{R}/R) \exp(-\frac{3}{8}\beta R^2)$$

with $n=2, l=0$. In the above definitions,

$$\mathbf{r}_{iD} = \mathbf{r}_i - \mathbf{R}_{TR}, \quad \mathbf{r}_{jD} = \mathbf{r}_j - \mathbf{R}_D \quad (18)$$

and

$$\mathbf{R} = \mathbf{R}_{TR} - \mathbf{R}_D \quad (19)$$

with

$$\mathbf{R}_{TR} = \frac{1}{3} \sum_{i=1}^3 \mathbf{r}_i, \quad \mathbf{R}_D = \frac{1}{2} \sum_{j=5}^6 \mathbf{r}_j. \quad (20)$$

A. The Normalization, Kinetic, and Potential Integrals

Once again, we exhibit only the general form of the various integrals, with the details presented in Appendix I. Now, the normalization factor is shown to be

$$N^2 = 5! \int (\psi_0 - 2\psi_1 + \psi_2)^* \psi_0 d\tau, \quad (21)$$

in which

$$\psi_0 = \psi(123; 56), \quad \psi_1 = \psi(523; 16), \quad \psi_2 = \psi(563; 12). \quad (22)$$

These definitions are analogous to those of Eq. (9), wherein, at this time, the first three slots describe a triton cluster and the last two positions pertain to the deuteron cluster.

The expression for the expectation value of the kinetic energy operator is somewhat more complicated due to the extra variational parameter $\bar{\alpha}$; however, it still can be subsumed in the form

$$\begin{aligned} \langle T \rangle = & (\hbar^2/2M)(2n\beta + 3\beta + 6\alpha + 3\bar{\alpha}) \\ & - 5!(\hbar^2/2M)(1/N^2) \int (\psi_0 - 2\psi_1 + \psi_2)^* \\ & \times (-2\alpha^2 \partial/\partial\alpha - 2\bar{\alpha}^2 \partial/\partial\bar{\alpha} - 2\beta^2 \partial/\partial\beta) \psi_0 d\tau \\ & - 5!(\hbar^2/2M)[n(n+1) - l(l+1)]/(1.2N^2) \\ & \times \int (\psi_0 - 2\psi_1 + \psi_2)^* (1/R^2) \psi_0 d\tau. \quad (23) \end{aligned}$$

Finally, the potential energy is computed and leads to the expression

$$\begin{aligned} \langle V \rangle = & (5!/N^2) \int \psi_0^* \{ w(6F_{12} + 4F_{15} + 2F_{56}) \\ & + b(F_{15} + 2F_{56}) \} \psi_0 d\tau \\ & - (5!/N^2) \int \psi_1^* \{ w(-4F_{15} + 4F_{23} + 8F_{16} + 16F_{12}) \\ & + b(-F_{15} - 2F_{23} - 3F_{26} + 8F_{16} + 4F_{12}) \} \psi_0 d\tau \\ & + (5!/N^2) \int \psi_2^* \{ w(4F_{12} + 8F_{13}) \\ & + b(3F_{15} + 4F_{12} - 4F_{13}) \} \psi_0 d\tau, \quad (24) \end{aligned}$$

with F_{ij} defined by Eq. (12). For this particular state, the spin-orbit potential does not contribute, whereas the Bartlett and Heisenberg forces contribute that part of the potential energy which multiplies b .

B. Numerical Analysis

Here too, we obtain an expression for the total energy of the system from which we must subtract the internal energies of the clusters to obtain the interaction energy. To this we add the Mang-Wild result for the energy of a triton cluster which can be cast in the analytic form of

$$E_{TR} = -8.48 + 8.60(1 - 1.41/y)^2 \text{ Mev}, \quad (25)$$

wherein we have again shifted the curve corresponding to their result to obtain the correct triton rms radius and binding energy. For this form, the discussion following Eq. (14) also applies. However, since the above expression is in rough agreement with the results

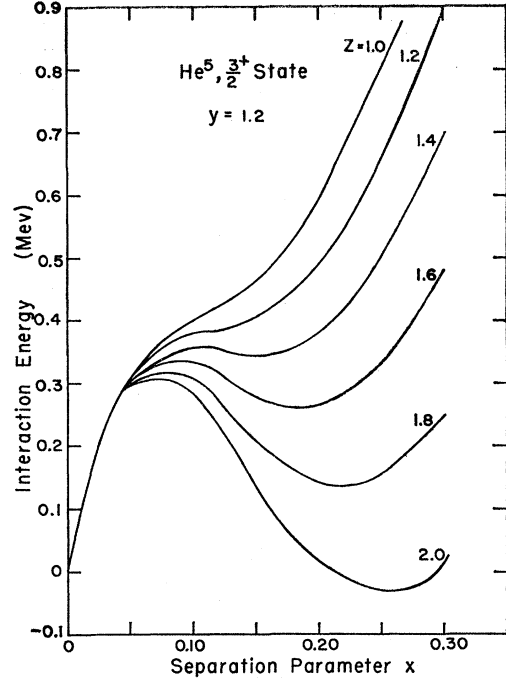


FIG. 3. Interaction energy as a function of the separation parameter for the $(\frac{3}{2}^+)$ state in He^5 with $y=1.2$.

of Ohmura et al.,²⁰ we feel that it should be reasonably valid. In Eq. (25), we have again made use of the definitions of Eq. (15). Also, for computational pur-

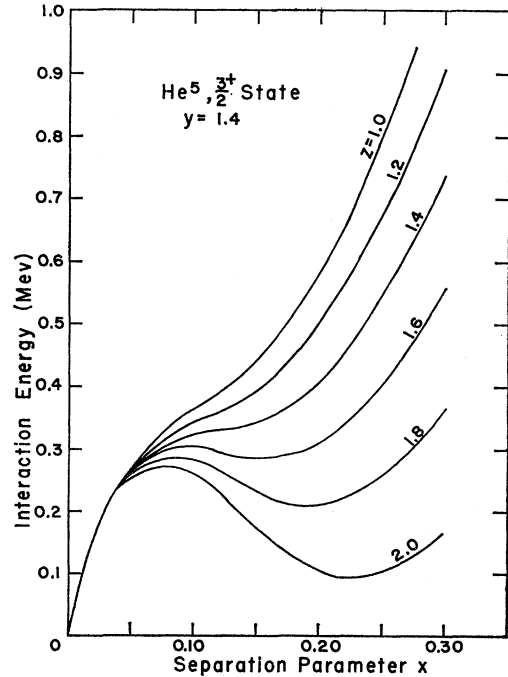


FIG. 4. Interaction energy as a function of the separation parameter for the $(\frac{3}{2}^+)$ state in He^5 with $y=1.4$.

²⁰ T. Ohmura, M. Morita, and M. Yamada, Progr. Theoret. Phys. (Kyoto) 15, 222 (1956); 17, 326 (1957); 22, 34 (1947).

poses, we have further defined

$$z = \bar{\alpha}/\alpha. \quad (26)$$

The deuteron cluster internal energy incorporated is that which is calculated with our Serber force of Eq. (7). The interaction energies as a function of x with y and z as parameters are plotted in the graphs of Figs. 3, 4, and 5. The occurrence of the relative minima indicates the presence of a resonant state. We note that these minima occur at small values of x which correspond to a large separations between the clusters, thus accounting for the large interaction radius encountered experimentally. It should further be noted that these values of x correspond to a large deviation from the usual shell model picture. The graphs in Fig. 6 show the departure of the interaction energy from the shell model value (obtained with $\beta = \alpha = \bar{\alpha}$) for several values of the width parameter y . We note that this energy difference is approximately 6 Mev. Finally, we have added the Coulomb energy which we have calculated without antisymmetrization; this is a justifiable procedure since the clusters are so well separated. The resultant total energy thus obtained for this state in He^5 is -8.26 Mev; the experimental value is -10.63 Mev. At this energy, the variational parameters are: $x=0.15$, $y=1.48$, $z=1.7$.

Also, we have determined the difference in excitation energies of the $(\frac{3}{2}^+)$ states in Li^6 and He^5 and found it to be 0.12 Mev, which is the present experimental value.³ This latter difference is, of course, nothing but a Coulomb effect.

IV. CONCLUSIONS AND DISCUSSIONS

We begin by discussing the negative parity states. The most obvious remark is that our results show that the $(\frac{1}{2}^-)$ state must have a large level width; as previously mentioned, this is in complete accord with the experimental situation. Also it should again be noted that a neutron-alpha configuration can lead to no resonant level other than the ground state and the first excited state. As for the difference between the experimental value and our theoretical prediction for the energy of the $(\frac{3}{2}^-)$ state, we should indicate that if we had used a wave function with a longer tail to describe the relative motion, our result would probably be improved. Also, it should be mentioned here that our simple Serber force is certainly not rigorously correct; hence we must keep this in mind as a possible source of discrepancy. Moreover, the uncertainty in the spin-orbit potential restricts our making a more complete analysis; however, we anticipate examining Li^6 and re-examining Li^7 to obtain an anchor on this potential. With this information, we can then make a more positive estimate of the energy of this state.

Of more interest is the $(\frac{3}{2}^+)$ level at 16.69 Mev. The results of our calculation definitely show that this

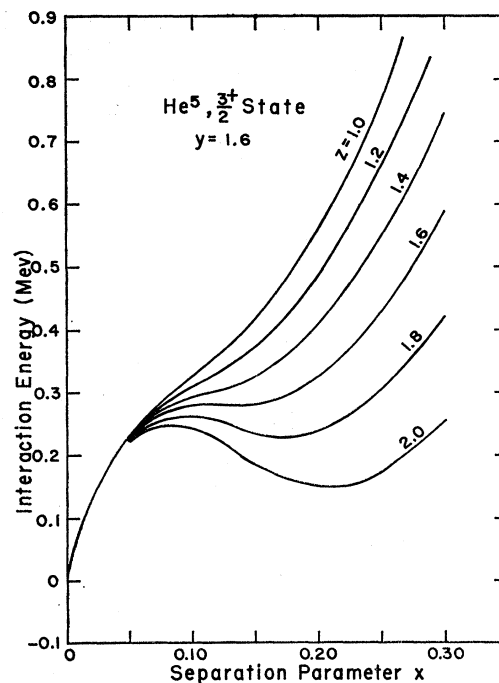


FIG. 5. Interaction energy as a function of the separation parameter for the $(\frac{3}{2}^+)$ state in He^5 with $y=1.6$.

level is a deuteron-triton configuration. The overestimate of the energy of this state is attributed to our rather poor choice of the deuteron cluster wave function, i.e., a simple Gaussian form. Using such a wave function to determine the binding energy of a free deuteron produces in this energy an error of approximately 2 Mev. However, if we use a wave function which is the

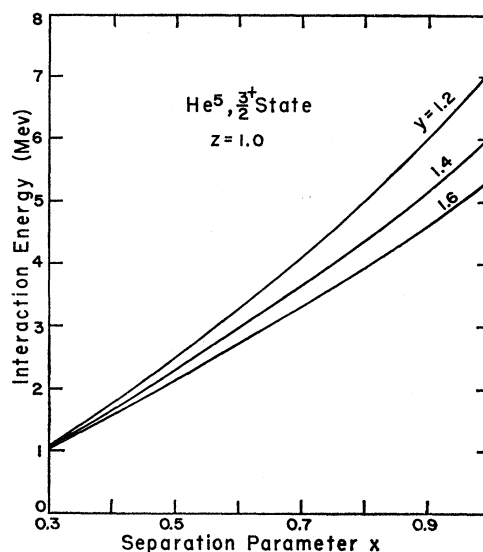


FIG. 6. Interaction energy as a function of the separation parameter for the $(\frac{3}{2}^+)$ state in He^5 , showing the effect of departure from the usual shell-model calculation.

sum of two Gaussians, the Serber potential then yields approximately the correct free deuteron binding energy. We, therefore, anticipate that if we had used the more appropriate wave function, we would have eliminated the major portion of the discrepancy. Unfortunately, the inclusion of the extra Gaussian term would complicate the analysis to such an extent that we do not feel that this extra work is warranted at the present time, especially so, since we can easily estimate the effect.

The occurrence of relative minima in our calculation not only allows for a determination of an upper bound to the energies of the various states, but also permits an estimate of the relative lifetimes of these states through an examination of the "tunnel effect." The results of such an investigation indicate that the width of the $(\frac{3}{2}^+)$ state is somewhat narrower than that of the ground state which is in agreement with the experimental situation. The obvious extension leads us to the presumption that changes in the cluster structure should be accompanied by abrupt changes in the level widths; that is, if in a sequence of levels in a given light nucleus, one finds that the tendency of ever increasing widths is suddenly interrupted by the presence of a much narrower one (which is quite generally the case), it is presupposed that the appropriate wave function has a completely different cluster structure which necessarily has a small transition probability to other configurations. One associates the systematic trend of widths with changes in the relative motion among the clusters only. This latter grouping of states was referred to as rotational levels in reference 2. This situation prevails in Be^8 , for instance, where we find that the first three levels, whose widths increase with excitation, can be described by merely changing the relative motion.¹ However, at 16.08 Mev the first narrow level occurs which, in our picture, should be described by an alpha cluster and a broken-up alpha cluster. An analogous situation occurs in Li^6 as well. Hence, from this discussion we note that the excitation

energy is not the determining factor in the level width of a state.

Another interesting point encountered in the study of He^5 and Li^5 lies in a comparison of the excitation energies of the $(\frac{3}{2}^+)$ states in this mirror pair. If the cluster structure of these states were the same as that of the ground state, it would be expected that He^5 would have the greater excitation energy—a situation which does not occur experimentally. However, if the excited states were deuteron-triton (He^3) configurations, which is actually the case, the reverse would occur. Experimentally, it has been determined that Li^5 has an excitation energy which is greater than that of He^5 by 0.12 Mev, the value which we arrive at. In general, we would expect an anomalous behavior of the Coulomb contribution to the excitation energies of isotopic spin multiplets whenever there is a change of cluster structure associated with these levels.²¹

From this investigation, we also note that our calculation indicates a strong need for a departure from the shell model. Such a departure can introduce great changes in the energy of a state as is seen in a rather spectacular fashion in the $(\frac{3}{2}^+)$ level and in a lesser manner in the $(\frac{3}{2}^-)$ state. We venture to say here that this effect might be partially responsible for the relatively low excitation energies of the second (0^+) levels in O^{16} and C^{12} .

Finally, we like to remark that our approximate manner of handling the hard core part of the nuclear two-body force can only be justified at the present moment by the relative success of our calculations and our belief that such saturating forces are only important in determining the internal energies of clusters in light nuclei. Certainly, if one extends this method to heavier nuclei, such an approximation is not expected to be valid. As has already been mentioned in I, this method probably would cease to yield reasonable results for $A > 12$; consequently, a more consistent way of handling the hard core must be sought.

APPENDIX I

In this appendix, we present the explicit evaluation of the expectation value of the Hamiltonian which is given by

$$E(\alpha, \beta) = \int \Psi^* H \Psi d\tau / \int \Psi^* \Psi d\tau. \quad (\text{A1})$$

In general, we shall need to evaluate expressions of the form $\int \Psi^* Q \Psi d\tau$. Specifically, for the alpha-nucleon configuration which we now consider, the terms which arise have the structure

$$Q_0 = \int \psi_0^* Q \psi_0 d\tau \quad (\text{A2})$$

and

$$Q_1 = \int \psi_1^* Q \psi_0 d\tau, \quad (\text{A3})$$

²¹ See CERN Report 59-23 (unpublished), reference 2.

or more explicitly,

$$Q_0 = 4^3 \int \exp\left(-\frac{\alpha}{2} \sum_{i=1}^4 r_{iD}^2 - \frac{2}{5}\beta R^2\right) R^n Y_{lm}^*(\mathbf{R}/R) Q(\mathbf{R}; \dots \mathbf{r}_{iD}) \exp\left(-\frac{\alpha}{2} \sum_{i=1}^4 r_{iD}^2 - \frac{2}{5}\beta R^2\right) \\ \times R^n Y_{lm}(\mathbf{R}/R) d\mathbf{R} d\mathbf{r}_{1D} d\mathbf{r}_{2D} d\mathbf{r}_{3D}, \quad (\text{A4})$$

and

$$Q_1 = 4^3 \int \exp\left[-\frac{\alpha}{2} \sum_{i=1}^4 r_{iD}^2 - \frac{2}{5}\beta R^2 - \frac{2}{5}\alpha(R'^2 - R^2)\right] R^n Y_{lm}^*(\mathbf{R}/R) \delta\left(\mathbf{R} + \frac{1}{4}\mathbf{R}' + \frac{5}{4}\mathbf{r}_{1D}\right) \\ \times Q(\mathbf{R}'; \dots \mathbf{r}_{iD} \dots) \exp\left[-\frac{\alpha}{2} \sum_{i=1}^4 r_{iD}^2 - \frac{2}{5}\beta R'^2\right] R'^n Y_{lm}(\mathbf{R}'/R') d\mathbf{R} d\mathbf{R}' d\mathbf{r}_{1D} d\mathbf{r}_{2D} d\mathbf{r}_{3D}, \quad (\text{A5})$$

where 4^3 is the Jacobian of the transformation from \mathbf{r}_i to \mathbf{r}_{iD} . To derive the results given by Eqs. (A4) and (A5), we made use of the definitions of Eqs. (3) and (9).

The normalization factor can be obtained by setting Q equal to unity in Eqs. (A4) and (A5). Integrating over the coordinates \mathbf{r}_{1D} , \mathbf{r}_{2D} , and \mathbf{r}_{3D} , we finally obtain

$$N^2 = 5!(A_0 - A_1), \quad (\text{A6})$$

with the no-exchange term

$$A_0 = 2^3 (\pi/\alpha)^{9/2} I_{2n+2}(\beta), \quad (\text{A7})$$

and the one-exchange term

$$A_1 = 4^3 \left(\frac{4}{5}\right)^3 \left(\frac{\pi^2}{3\alpha^2}\right)^{\frac{3}{2}} J_{n+2, n+2, l} \left(\frac{17}{15}\alpha + \beta, \frac{16}{15}\alpha, \frac{17}{15}\alpha + \beta\right), \quad (\text{A8})$$

where

$$I_\mu(p) = \int R^\mu \exp(-\frac{4}{5}pR^2) |Y_{lm}(\mathbf{R}/R)|^2 d\mathbf{R} d\Omega, \quad (\text{A9})$$

and

$$J_{\mu, \nu, l}(p, q, s) = \int R'^\mu R^\nu \exp\left[-\frac{2}{5}(pR'^2 + q\mathbf{R}' \cdot \mathbf{R} + sR^2)\right] Y_{lm}(\mathbf{R}'/R') Y_{lm}^*(\mathbf{R}/R) d\mathbf{R}' d\mathbf{R} d\Omega' d\Omega. \quad (\text{A10})$$

In Eq. (A8), the factor $(\frac{4}{5})^3$ arises from the delta function in Eq. (A5).

Both I_μ and $J_{\mu, \nu, l}$ are rather elementary integrals and can be readily integrated by making use of the existing tables on Mellin transforms and Laplace transforms²² to yield the following expressions:

$$I_\mu(p) = \frac{\sqrt{\pi}}{2^{\mu/2+1}} \left(\frac{4}{5}p\right)^{-(\mu+1)/2} (\mu-1)!!, \quad (\text{A11})$$

$$J_{\mu, \nu, l}(p, q, s) = \frac{(-1)^l \pi^{\frac{3}{2}}}{2^{l+1}} \left(\frac{5}{2}\right)^{(\mu+\nu+2)/2} \frac{q^l}{p^{(\mu+l+1)/2} s^{(\nu+l+1)/2}} \frac{\Gamma((\mu+l+1)/2) \Gamma((\nu+l+1)/2)}{\Gamma(l+\frac{3}{2})} \\ \times {}_2F_1\left(\frac{\mu+l+1}{2}, \frac{\nu+l+1}{2}; l+\frac{3}{2}; \frac{q^2}{4ps}\right), \quad (\text{A12})$$

where $(\mu-1)!! \equiv (\mu-1)(\mu-3)(\mu-5)\dots$, and ${}_2F_1$ is the hypergeometric function.

In arriving at Eq. (A12), use is made of the expansion,²³

$$\exp(-\frac{2}{5}q\mathbf{R}' \cdot \mathbf{R}) = 4\pi \sum_{lm} (-1)^l \left(\frac{5\pi}{4qR'R}\right)^{\frac{1}{2}} I_{l+\frac{1}{2}}(\frac{2}{5}qR'R) Y_{lm}^*(\mathbf{R}'/R') Y_{lm}(\mathbf{R}/R), \quad (\text{A13})$$

where $I_{l+\frac{1}{2}}(\frac{2}{5}qR'R)$ are Bessel functions of half integral order of the imaginary argument $\frac{2}{5}iqR'R$.

For the expectation value of the kinetic energy, we have for Q those operators which are expressed explicitly

²² A. Erdelyi, W. Magnus, F. Oberhettinger, and F. G. Tricomi, *Tables of Integral Transforms* (McGraw-Hill Book Company, Inc., New York, 1954), Vol. 1, p. 146 and p. 334.

²³ W. Magnus and F. Oberhettinger, *Function of Mathematical Physics* (Chelsea Publishing Company, New York, 1954).

in Eq. (10). Inserting them into Eqs. (A4) and (A5), we then obtain

$$\langle T \rangle = (\hbar^2/2M)(2n\beta + 3\beta + 9\alpha) - 5! \frac{\hbar^2}{2M} \frac{1}{N^2} (C_0 - C_1) - 5! \frac{\hbar^2}{2M} \frac{n(n+1) - l(l+1)}{0.8N^2} (B_0 - B_1), \quad (\text{A14})$$

with

$$B_0 = 2^3 (\pi/\alpha)^{9/2} I_{2n}(\beta), \quad B_1 = 4^3 \left(\frac{4}{5}\right)^3 \left(\frac{\pi^2}{3\alpha^2}\right)^{3/2} J_{n, n+2, l} \left(\frac{17}{15}\alpha + \beta, \frac{16}{15}\alpha, \frac{17}{15}\alpha + \beta\right), \quad (\text{A15})$$

and

$$C_0 = \frac{1}{2}(2n\beta + 3\beta + 9\alpha)A_0, \quad C_1 = [(n+6)\alpha + \Lambda((17/15)\alpha + \beta, (16/15)\alpha)]A_1, \quad (\text{A16})$$

where

$$\Lambda(p, q) = (2n+3) \frac{\beta(\beta-\alpha)}{p} \left(1 - \frac{q^2}{4p^2}\right)^{-1} \frac{{}_2F_1\left(-\frac{n-l+2}{2}, -\frac{n-l}{2}; -\frac{2n+3}{2}; 1 - \frac{q^2}{4p^2}\right)}{{}_2F_1\left(-\frac{n-l}{2}, -\frac{n-l}{2}; -\frac{2n+1}{2}; 1 - \frac{q^2}{4p^2}\right)}, \quad (\text{A17})$$

To arrive at Eq. (A16), we have used the fact that in our case, $(n-l)$ is an even integer greater than or equal to zero.

Next, the expectation value for the potential energy operator as given by Eq. (11) can be obtained by inserting the appropriate functions for Q into Eqs. (A4) and (A5); the results for the individual contributions are

$$\begin{aligned} F_{12}^0 &= -V_0 \left\{ \left(\frac{\alpha}{\alpha+2\kappa} \right)^{3/2} A_0 \right\}, \\ F_{15}^0 &= -V_0 \left\{ 4^3 \left(\frac{\pi}{\alpha} \right)^3 \left(\frac{\pi}{3\kappa+4\alpha} \right)^{3/2} I_{2n+2} \left(\beta + \frac{5\alpha\kappa}{4\alpha+3\kappa} \right) \right\}, \\ F_{12}^1 &= -V_0 \left\{ 4^3 \left(\frac{4}{5} \right)^3 \left[\frac{\pi^2}{\alpha(3\alpha+2\kappa)} \right]^{3/2} J_{n+2, n+2, l} \left(\frac{17\alpha+14\kappa}{15\alpha+10\kappa}\alpha + \beta, \frac{16\alpha+32\kappa}{15\alpha+10\kappa}\alpha, \frac{17\alpha+54\kappa}{15\alpha+10\kappa}\alpha + \beta \right) \right\}, \\ F_{23}^1 &= -V_0 \left\{ \left(\frac{\alpha}{\alpha+2\kappa} \right)^{3/2} A_1 \right\}, \\ F_{15}^1 &= -V_0 \left\{ 4^3 \left(\frac{4}{5} \right)^3 \left(\frac{\pi^2}{3\alpha^2} \right)^{3/2} J_{n+2, n+2, l} \left(\frac{17}{15}\alpha + \beta + \frac{8}{5}\kappa, \frac{16}{15}\alpha - \frac{16}{15}\kappa, \frac{17}{15}\alpha + \beta + \frac{8}{5}\kappa \right) \right\}, \end{aligned} \quad (\text{A18})$$

and

$$\begin{aligned} G_{15}^0 &= -V_{LS} \left(\frac{5}{4} \right) 4^3 \left\{ \left(\frac{\pi}{\alpha} \right)^3 \left(\frac{\pi}{3\lambda+4\alpha} \right)^{3/2} I_4 \left(\beta + \frac{5\alpha\lambda}{4\alpha+3\lambda} \right) + \left(\frac{\pi^2}{3\alpha^2} \right)^{3/2} J_{331} \left(2\beta + \frac{5}{2}\lambda, 5\lambda, \frac{10}{3}\alpha + \frac{5}{2}\lambda \right) \right\}, \\ G_{15}^1 &= -V_{LS} \left(\frac{5}{4} \right) 4^3 \left(\frac{\pi^2}{3\alpha^2} \right)^{3/2} \left\{ \left(\frac{4}{5} \right)^3 J_{331} \left(\frac{17}{15}\alpha + \beta + \frac{8}{5}\lambda, \frac{16}{15}\alpha - \frac{16}{15}\lambda, \frac{17}{15}\alpha + \beta + \frac{8}{5}\lambda \right) \right. \\ &\quad + 4^3 J_{331} \left(15\alpha + 17\beta + 40\lambda, 40\alpha + 40\beta + 80\lambda, \frac{85}{3}\alpha + 25\beta + 40\lambda \right) \\ &\quad + \frac{4}{15} \left(\frac{4}{5} \right)^4 (\alpha - \beta) \left[J_{442} \left(\frac{17}{15}\alpha + \beta + \frac{8}{5}\lambda, \frac{16}{15}\alpha - \frac{16}{15}\lambda, \frac{17}{15}\alpha + \beta + \frac{8}{5}\lambda \right) \right. \\ &\quad \left. \left. - J_{440} \left(\frac{17}{15}\alpha + \beta + \frac{8}{5}\lambda, \frac{16}{15}\alpha - \frac{16}{15}\lambda, \frac{17}{15}\alpha + \beta + \frac{8}{5}\lambda \right) \right] \right\}, \end{aligned} \quad (\text{A19})$$

$$\begin{aligned}
G_{25}^1 = & -V_{LS}\left(\frac{4}{3}\right)^2 4^3 \left\{ \left[\frac{\pi^2}{\alpha(3\alpha+2\lambda)} \right]^{\frac{3}{2}} J_{331} \left(\frac{17\alpha+14\lambda}{15\alpha+10\lambda} \alpha+\beta, \frac{16\alpha+32\lambda}{15\alpha+10\lambda} \alpha, \frac{17\alpha+54\lambda}{15\alpha+10\lambda} \alpha+\beta \right) + \left[\frac{\pi^2}{\alpha[(23/25)\alpha+\frac{4}{5}\beta+2\lambda]} \right]^{\frac{3}{2}} \right. \\
& \times J_{331} \left(\frac{25\alpha^2+51\alpha\beta+20\beta^2+10\lambda(7\alpha+5\beta)}{23\alpha+20\beta+50\lambda}, -\frac{40\alpha^2+40\alpha\beta+160\alpha\lambda}{23\alpha+20\beta+50\lambda}, \frac{85\alpha^2+75\alpha\beta+10\lambda(27\alpha+5\beta)}{23\alpha+20\beta+50\lambda} \right) \\
& - \frac{1}{3} \left(\frac{4}{3} \right)^2 \left[\frac{\pi^2}{\alpha(3\alpha+2\lambda)} \right]^{\frac{3}{2}} \frac{\alpha}{3\alpha+2\lambda} (\alpha-\beta) \left[J_{442} \left(\frac{17\alpha+14\lambda}{15\alpha+10\lambda} \alpha+\beta, \frac{16\alpha+32\lambda}{15\alpha+10\lambda} \alpha, \frac{17\alpha+54\lambda}{15\alpha+10\lambda} \alpha+\beta \right) \right. \\
& \left. \left. - J_{440} \left(\frac{17\alpha+14\lambda}{15\alpha+10\lambda} \alpha+\beta, \frac{16\alpha+32\lambda}{15\alpha+10\lambda} \alpha, \frac{17\alpha+54\lambda}{15\alpha+10\lambda} \alpha+\beta \right) \right] \right\}. \quad (A19)
\end{aligned}$$

In the above expressions, the superscripts 0 and 1 refer to no-exchange and one-exchange, respectively. We like to point out here that Eq. (A18) also applies to the cases with $n=2$ and $l=0, 2$, while Eq. (A19) is only correct for the case with $n=l=1$.

Next we turn to the deuteron-triton configuration, i.e., the $(\frac{3}{2}^+)$ state of He⁵. Using the previously illustrated technique, we obtain for the normalization factor the expression

$$N^2 = A_0 - 2A_1 + A_2, \quad (A20)$$

with

$$\begin{aligned}
A_0 &= 6^3 \left(\frac{\pi^2}{3\alpha^2} \right)^{\frac{3}{2}} \left(\frac{\pi}{2\bar{\alpha}} \right)^{\frac{3}{2}} K_{2n+2}(\beta), \\
A_1 &= 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{\alpha(3\alpha+4\bar{\alpha})} \right]^{\frac{3}{2}} L_{n+2, n+2, l} \left(\frac{\omega}{\sigma} + \beta, -\frac{\xi}{\sigma}, \frac{\omega}{\sigma} + \beta \right), \\
A_2 &= 6^3 \left(\frac{6}{5} \right)^3 \left(\frac{\pi}{\alpha+\bar{\alpha}} \right)^3 L_{n+2, n+2, l} \left(\frac{13}{5} \alpha + \beta, \frac{24}{5} \alpha, \frac{13}{5} \alpha + \beta \right),
\end{aligned} \quad (A21)$$

wherein

$$\sigma = 15\alpha + 20\bar{\alpha}, \quad \omega = 6\alpha^2 + 25\alpha\bar{\alpha} + 6\bar{\alpha}^2, \quad \xi = 12\alpha^2 + 12\bar{\alpha}^2, \quad (A22)$$

and

$$K_\mu(p) = \int R^\mu \exp\left(-\frac{6}{5}pR^2\right) |Y_{lm}(\mathbf{R}/R)|^2 dR d\Omega, \quad (A23)$$

$$L_{\mu\nu l}(p, q, s) = \int R'^\mu R^\nu \exp\left[-\frac{3}{5}(pR'^2 + q\mathbf{R}' \cdot \mathbf{R} + sR^2)\right] Y_{lm}(\mathbf{R}'/R') Y_{lm}^*(\mathbf{R}/R) dR' dR d\Omega' d\Omega.$$

Similarly, for the kinetic energy, we have

$$\langle T \rangle = (\hbar^2/2M)(2n\beta + 3\beta + 6\alpha + 3\bar{\alpha}) - 5! \frac{\hbar^2}{2M N^2} (C_0 - 2C_1 + C_2) - 5! \frac{\hbar^2}{2M} \frac{n(n+1) - l(l+1)}{1.2N^2} (B_0 - 2B_1 + B_2), \quad (A23)$$

in which the B 's and the C 's are defined by the following integrals:

$$\begin{aligned}
B_0 &= 6^3 \left(\frac{\pi^2}{3\alpha^2} \right)^{\frac{3}{2}} \left(\frac{\pi}{2\bar{\alpha}} \right)^{\frac{3}{2}} K_{2n}(\beta), \\
B_1 &= 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{\alpha(3\alpha+4\bar{\alpha})} \right]^{\frac{3}{2}} L_{n, n+2, l} \left(\frac{\omega}{\sigma} + \beta, -\frac{\xi}{\sigma}, \frac{\omega}{\sigma} + \beta \right), \\
B_2 &= 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi}{\alpha+\bar{\alpha}} \right]^3 L_{n, n+2, l} \left(\frac{13}{5} \alpha + \beta, \frac{24}{5} \alpha, \frac{13}{5} \alpha + \beta \right), \\
C_0 &= \frac{2n\beta + 3\beta + 6\alpha + 3\bar{\alpha}}{2} A_0,
\end{aligned} \quad (A24)$$

$$C_1 = \left\{ \left[\frac{3}{2}\alpha - (n + \frac{3}{2}) \frac{3\alpha^2 + 4\bar{\alpha}^2}{3\alpha + 4\bar{\alpha}} + 2(n+3) \frac{\alpha^3 + \bar{\alpha}^3}{\alpha^2 + \bar{\alpha}^2} \right] \right. \\ \left. + \left[1 - \frac{12\bar{\alpha}(\bar{\alpha} - \alpha)}{\beta(\beta - \alpha)\sigma\xi} [25\alpha\bar{\alpha}^2 - 25\alpha^3 + 10\beta(2\bar{\alpha} - \alpha)(\bar{\alpha} + 2\alpha)] \right] \Lambda \left(\frac{\omega}{\sigma} + \beta, \frac{\xi}{\sigma} \right) \right\} A_1, \\ C_2 = \left\{ \left[(n+3)\alpha + 3 \frac{\alpha^2 + \bar{\alpha}^2}{\alpha + \bar{\alpha}} \right] + \Lambda \left(\frac{13}{5}\alpha + \beta, \frac{24}{5}\alpha \right) \right\} A_2,$$

with Λ defined by Eq. (A17).

Finally, for the various terms of the potential energy, we have [see Eq. (24)]

$$F_{12}^0 = -V_0 \left\{ \left(\frac{\alpha}{\alpha + 2\kappa} \right)^{\frac{3}{2}} A_0 \right\} \\ F_{16}^0 = -V_0 \left\{ 6^3 \left(\frac{\pi}{\alpha} \right)^{\frac{3}{2}} \left[\frac{\pi^2}{6\alpha\bar{\alpha} + \kappa(3\alpha + 4\bar{\alpha})} \right]^{\frac{3}{2}} K_{2n+2} \left(\beta + \frac{5\alpha\bar{\alpha}\kappa}{6\alpha\bar{\alpha} + \kappa(3\alpha + 4\bar{\alpha})} \right) \right\}, \\ F_{56}^0 = -V_0 \left\{ \left(\frac{\bar{\alpha}}{\bar{\alpha} + 2\kappa} \right)^{\frac{3}{2}} A_0 \right\}, \\ F_{16}^1 = -V_0 \left\{ 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{\alpha(3\alpha + 4\bar{\alpha})} \right]^{\frac{3}{2}} L_{n+2, n+2, l} \left(\frac{\omega}{\sigma} + \beta + \frac{12}{5}\kappa, -\frac{\xi}{\sigma} - \frac{24}{5}\kappa, \frac{\omega}{\sigma} + \beta + \frac{12}{5}\kappa \right) \right\}, \\ F_{23}^1 = -V_0 \left\{ \left(\frac{\alpha}{\alpha + 2\kappa} \right)^{\frac{3}{2}} A_1 \right\}, \\ F_{16}^1 = -V_0 \left\{ 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{\alpha(3\alpha + 4\bar{\alpha} + 8\kappa)} \right]^{\frac{3}{2}} L_{n+2, n+2, l} \left(\frac{\omega + 80\alpha\kappa + 24\bar{\alpha}\kappa}{\sigma + 40\kappa} + \beta, -\frac{\xi + 48\bar{\alpha}\kappa}{\sigma + 40\kappa}, \frac{\omega + 20\alpha\kappa + 24\bar{\alpha}\kappa}{\sigma + 40\kappa} + \beta \right) \right\}, \\ F_{26}^1 = -V_0 \left\{ 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{3\alpha^2 + 4\alpha\bar{\alpha} + \kappa(2\alpha + 2\bar{\alpha})} \right]^{\frac{3}{2}} \right. \\ \left. \times L_{n+2, n+2, l} \left(\frac{\alpha\omega + \kappa(\alpha + \bar{\alpha})(29\alpha + 3\bar{\alpha})}{\alpha\sigma + 10\kappa(\alpha + \bar{\alpha})} + \beta, -\frac{\alpha\xi - 6\kappa(\alpha + \bar{\alpha})(7\alpha - \bar{\alpha})}{\alpha\sigma + 10\kappa(\alpha + \bar{\alpha})}, \frac{\alpha\omega + \kappa(\alpha + \bar{\alpha})(29\alpha + 3\bar{\alpha})}{\alpha\sigma + 10\kappa(\alpha + \bar{\alpha})} + \beta \right) \right\}, \\ F_{12}^1 = -V_0 \left\{ 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{3\alpha^2 + 4\alpha\bar{\alpha} + 2\kappa(3\alpha + \bar{\alpha})} \right]^{\frac{3}{2}} \right. \\ \left. \times L_{n+2, n+2, l} \left(\frac{\alpha\omega + \kappa(21\alpha^2 + 80\alpha\bar{\alpha} + 3\bar{\alpha}^2)}{\alpha\sigma + 10\kappa(3\alpha + \bar{\alpha})} + \beta, -\frac{\alpha\xi + 6\kappa(7\alpha^2 + \bar{\alpha}^2)}{\alpha\sigma + 10\kappa(3\alpha + \bar{\alpha})}, \frac{\alpha\omega + \kappa(21\alpha^2 + 20\alpha\bar{\alpha} + 3\bar{\alpha}^2)}{\alpha\sigma + 10\kappa(3\alpha + \bar{\alpha})} + \beta \right) \right\}, \\ F_{15}^2 = -V_0 \left\{ 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{(\alpha + \bar{\alpha})(2\kappa + \alpha + \bar{\alpha})} \right]^{\frac{3}{2}} \right. \\ \left. \times L_{n+2, n+2, l} \left(\frac{26\alpha(\alpha + \bar{\alpha}) + 2\kappa(29\alpha + 3\bar{\alpha})}{10(\alpha + \bar{\alpha}) + 20\kappa} + \beta, \frac{48\alpha(\alpha + \bar{\alpha}) + 12\kappa(7\alpha - \bar{\alpha})}{10(\alpha + \bar{\alpha}) + 20\kappa}, \frac{26(\alpha + \bar{\alpha}) + 2\kappa(29\alpha + 3\bar{\alpha})}{10(\alpha + \bar{\alpha}) + 20\kappa} + \beta \right) \right\}, \\ F_{12}^2 = -V_0 \left\{ \left(\frac{\alpha + \bar{\alpha}}{\alpha + \bar{\alpha} + 4\kappa} \right)^{\frac{3}{2}} A_2 \right\}, \\ F_{13}^2 = -V_0 \left\{ 6^3 \left(\frac{6}{5} \right)^3 \left[\frac{\pi^2}{(\alpha + \bar{\alpha})(\alpha + \bar{\alpha} + \kappa)} \right]^{\frac{3}{2}} \right. \\ \left. \times L_{n+2, n+2, l} \left(\frac{26\alpha(\alpha + \bar{\alpha}) + 2\kappa(25\alpha + 12\bar{\alpha})}{10(\alpha + \bar{\alpha}) + 10\kappa} + \beta, \frac{48\alpha(\alpha + \bar{\alpha}) + 24\kappa(5\alpha + 3\bar{\alpha})}{10(\alpha + \bar{\alpha}) + 10\kappa}, \frac{26\alpha(\alpha + \bar{\alpha}) + 2\kappa(40\alpha + 27\bar{\alpha})}{10(\alpha + \bar{\alpha}) + 10\kappa} + \beta \right) \right\}, \tag{A25}$$

where the superscript 2 refers to the two-exchange terms.