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Three-Body Nuclear Problem with Repulsive Core Forces*†

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A variational calculation of the binding energy of the triton has been carried out using the Gartenhaus potential. The results indicate that this potential leads to an unbound ground state of the three-nucleon system; this result is attributable to the even-parity tensor potential which is relatively large in magnitude compared to the weakly attractive even-parity central potential. Since this property is also a characteristic of the Signell-Marshak potential, it too should lead to an unbound triton.

I. INTRODUCTION

DURING the past few years, a great amount of effort has been expended in obtaining repulsive-core nucleon-nucleon potentials which are consistent with a wide range of two-body data. A number of such potentials have been found which lead to good agreement with experiment.¹⁻⁴ While repulsive-core potentials may be treated in a straightforward manner in the two-body problem, they complicate considerably the three- and four-body nuclear problem; such systems have traditionally acted as critical tests for two-body potentials. Aside from calculations done with purely central hard-core forces,^{5,6} only Derrick and Blatt⁷ have heretofore calculated the binding energy of the triton with a realistic potential. Using Monte Carlo methods, they have found that the Gammel-Thaler potential apparently leads to a ground-state energy for the triton that is in the continuum region, $E \approx +2$ Mev.

In this paper the results of a variational calculation using the Gartenhaus potential² will be presented which indicate that this potential also predicts an unbound ground state for the triton. The Gartenhaus potential

is known to be inadequate for all but the lowest energies⁸ and it has been modified in a significant manner by Signell and Marshak^{4,9,10} to obtain agreement with scattering data up to 150 Mev. These extensive modifications were not included in the present calculation for several reasons: The most important change is the addition of a strong spin-orbit term to the potential. However, the matrix elements of a spin-orbit potential acting between two S states or an S and a D state vanish; the matrix element of a spin-orbit potential between the principal S and the principal P state (these states are defined in the next section) also is zero. Since the totally symmetric S state has by far the lowest kinetic energy, it should predominate in the ground state of the triton and any term in the nuclear potential which cannot couple the other important states directly to it can have little effect on the total energy. Signell and Marshak suggest making the odd-parity central potentials less attractive by setting them equal to zero in the core regions and at the same time making the positive cores of the even-parity central potentials more repulsive. They have not defined these changes quantitatively but, as will be discussed later, decreasing the strength of the attractive central potential relative to the tensor should raise the total energy of the triton. In view of the latter point, it is felt that the results of the calculation reported here are characteristic of the Signell-Marshak potential as well as of that of Gartenhaus.

All of the calculations reported in this paper have been carried out using the more attractive singlet even-parity potential, ${}^1V_e^+$, of the two given by Gartenhaus.

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¹ Supplement No. 3, *Prog. of Theor. Phys.* (1956).

² S. Gartenhaus, *Phys. Rev.* **100**, 900 (1955).

³ J. L. Gammel and R. M. Thaler, *Phys. Rev.* **107**, 291 (1957); **107**, 1359 (1957).

⁴ P. S. Signell and R. E. Marshak, *Phys. Rev.* **109**, 1229 (1958).

⁵ T. Kikuta, M. Morita, and M. Yamada, *Progr. Theoret. Phys. (Kyoto)* **15**, 122 (1956).

⁶ H. Mang and W. Wild, *Z. Physik* **154**, 181 (1959).

⁷ G. H. Derrick and J. M. Blatt, *Nuclear Phys.* **8**, 310 (1958); G. H. Derrick, thesis, University of Sydney, 1959 (unpublished); G. H. Derrick, *Nuclear Phys.* **16**, 405 (1960); G. H. Derrick and J. M. Blatt, *Nuclear Phys.* **17**, 67 (1960).

⁸ J. L. Gammel and R. M. Thaler, *Phys. Rev.* **103**, 1874 (1956).

⁹ P. S. Signell and R. E. Marshak, *Phys. Rev.* **106**, 832 (1957).

¹⁰ P. S. Signell, R. Zinn, and R. E. Marshak, *Phys. Rev. Letters* **1**, 416 (1958).

II. ENERGY CALCULATION

The ground states of the two mirror nuclei H^3 and He^3 have a total angular momentum of $\frac{1}{2}$. The ground states can thus be completely represented as a linear combination of S , P , and D states, each coupled to the spins of the three nucleons to give $J=\frac{1}{2}$. Gerjuoy and Schwinger¹¹ were the first to list appropriate states in terms of operators constructed from the relative position vectors and spin operators acting on arbitrary scalar functions of the nucleon coordinates. Sachs¹² has listed 8 linearly independent states of essentially the same form but has added isotopic-spin functions, the total isotopic spin being taken to be $\frac{1}{2}$. More recently, Derrick⁷ has shown that one S and one P state have been omitted in the listing by Sachs. However, neither of these two states is expected to be present to an appreciable extent in the triton ground state.

In the present calculation the triton functions listed by Sachs were used. Of the eight linearly independent functions, three can be expected to be the most important because they contain the relative position vectors to lower powers than do the other states of the same orbital angular momentum. This means they are more smooth varying functions of nucleon position and can be expected to have lower kinetic energy. The three "principal" S , P , and D states are:

$$\begin{aligned} {}^2S: \Psi_1^{m,t} &= [\varphi^m \bar{\eta}^t - \bar{\varphi}^m \eta^t] f_1(\alpha_1, r_{ij}), \\ {}^2P: \Psi_3^{m,t} &= \{ [12i\sigma_3 \eta^t + (i\sigma_{12} + \sigma_{12} \times \sigma_3) \eta^{-t}] \\ &\quad \cdot [\mathbf{r} \times \boldsymbol{\rho}] \} \varphi^m f_3(\alpha_3, r_{ij}), \quad (1) \\ {}^2D: \Psi_7^{m,t} &= \{ \frac{1}{2} [(\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_3 \cdot \boldsymbol{\rho}) + (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\rho})(\boldsymbol{\sigma}_3 \cdot \mathbf{r}) \\ &\quad - \frac{2}{3}(\boldsymbol{\rho} \cdot \mathbf{r})(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_3)] \eta^{-t} - [(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\rho})(\boldsymbol{\sigma}_3 \cdot \boldsymbol{\rho}) \\ &\quad - 3(\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_3 \cdot \mathbf{r}) - \frac{1}{3}(\rho^2 - 3r^2)(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_3) \eta^t] \} \\ &\quad \times \varphi^m f_7(\alpha_7, r_{ij}). \end{aligned}$$

φ^m and η^t are, respectively, three-particle spin and isotopic-spin functions with total spin and isotopic spin $\frac{1}{2}$ which are antisymmetric in nucleons 1 and 2. $\bar{\varphi}^m$ and $\bar{\eta}^t$ are corresponding functions which are symmetric in 1 and 2. The two relative position vectors are defined as $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\boldsymbol{\rho} = \mathbf{r}_1 + \mathbf{r}_2 - 2\mathbf{r}_3$. The $f_k(\alpha_k, r_{ij})$ are, in general, arbitrary scalar functions which are symmetric under the interchange of any two nucleons. In the present calculation they were given the form

$$f_i = (r_{12} r_{23} r_{13})^n \exp[-\alpha_i(r_{12} + r_{23} + r_{13})]. \quad (2)$$

This form, with n an integer and α_i a variational parameter, is the one which satisfies the boundary conditions and is easiest to handle. As usual, $f_i \rightarrow 0$ for any $r_{ij} \rightarrow \infty$ and, because of the strongly repulsive cores of the Gartenhaus even-parity central potential, $f_i = 0$ for any $r_{ij} = 0$. For $i=7$, n was chosen to be 1 while for $i=1$ it was taken to be 1 (case A) and 2 (case

B). If one writes the ground state as

$$\begin{aligned} \Psi^{m,t} &= A_1 \Psi_1^{m,t} + A_3 \Psi_3^{m,t} + A_7 \Psi_7^{m,t}, \\ |A_1|^2 + |A_3|^2 + |A_7|^2 &= 1, \end{aligned} \quad (3)$$

and divides the Hamiltonian into a kinetic and potential energy part, $H = T + V$, the expectation value of the energy in the ground state is given by (omitting all terms identically equal to zero)

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= |A_1|^2 \langle \Psi_1 | T + V | \Psi_1 \rangle + |A_3|^2 \langle \Psi_3 | T + V | \Psi_3 \rangle \\ &\quad + |A_7|^2 \langle \Psi_7 | T + V | \Psi_7 \rangle + 2 \operatorname{Re} A_1^* A_7 \langle \Psi_1 | V_T | \Psi_7 \rangle \\ &\quad + 2 \operatorname{Re} A_3^* A_7 \langle \Psi_3 | V_T | \Psi_7 \rangle. \end{aligned} \quad (4)$$

In the above, V_T is the tensor potential. Neither a central nor a tensor potential can couple an S state to a P state so Ψ_3 cannot be coupled to Ψ_1 by the Gartenhaus potential. Therefore, Ψ_3 was omitted in the present calculation. The question arises of whether Ψ_3 could become important when a strong spin-orbit force is present, as it is in the Signell-Marshak potential. The answer is no because the $\mathbf{L} \cdot \mathbf{S}$ operator contains the factor $\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2$,¹³ which is always acting to either the right or left on φ^m for which the identity $\boldsymbol{\sigma}_1 \varphi^m \equiv -\boldsymbol{\sigma}_2 \varphi^m$ obtains.

The total energy was computed¹⁴ for a wide range of values of α_1 and α_7 and no minimum in the energy was found for the trial wave functions of cases A and B. However, for any fixed value of α_7 there is a value of α_1 for which a relative minimum exists. That is to say, there is a trough in the surface $E(\alpha_1, \alpha_7)$ running towards the origin. The total energy as a function of these values of α_1 is shown in Fig. 1.

At the same time, a two-body trial wave function with S - and D -state components, whose radial parts are given by

$$f_S = r_{12} \exp(-\alpha_S r_{12}), \quad f_D = r_{12} \exp(-\alpha_D r_{12}), \quad (5)$$

was used in a variational calculation of the deuteron total energy, again using the Gartenhaus potential. A definite minimum energy of +0.65 Mev was found. This value is to be compared to the experimental value of -2.226 Mev to which the Gartenhaus potential has been fitted. This difference corresponds to an error of about 10% in the potential energy and indicates there is likely to be an error of comparable size in our triton potential energy elements.

It seems clear that the difficulty stems from the relatively slow change of the S -state trial wave function in the core region as compared to the potential itself. The repulsive core should act more or less as a boundary condition and the wave function should fall off so rapidly that there is very little positive contribution to the potential energy. To check on this, the positive cores of the central potentials were set equal to zero, and all the calculations repeated. As a result, the

¹¹ E. Gerjuoy and J. Schwinger, Phys. Rev. **61**, 138 (1942).

¹² R. G. Sachs, *Nuclear Theory* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1953), Chap. 8.

¹³ Because of the complete antisymmetry of $\Psi^{m,t}$ only the $V(12)$ term need be calculated.

¹⁴ See Appendix for details.

deuteron energy was lowered to -4.83 Mev while a minimum of $+8.18$ Mev appeared for the triton trial function of case A. On the other hand, no minimum was found with the trial function of case B. The minimum of $+8.18$ Mev is produced by a change of about -12 Mev in the expectation value of H in the S state as compared with its value with the repulsive core present. This indicates that the wave functions are indeed deficient in the manner mentioned above.

Since our trial wave functions are believed to be very inadequate in the core region when used with the Gartenhaus potential, our conclusions concerning its consistency with the experimental energy of the triton can best be obtained by considering the value of the energy calculated upon setting the repulsive cores equal to zero and using the same form trial function. The minimum of $+8.18$ Mev represents an estimate of the lowest eigenvalue to the three-nucleon problem with the boundary conditions, $\Psi(r_{ij})=0$ for any $r_{ij} \rightarrow \infty$, $\Psi(r_{ij})=0$ for any $r_{ij}=0$, and a potential the same as the Gartenhaus except for the removal of the repulsive central cores. The exact lowest eigenvalue to this altered problem must be considerably lower than the energy predicted by the actual Gartenhaus potential. (For example, the estimate of the deuteron energy is already 2.6 Mev lower than the known eigenvalue with the complete Gartenhaus potential.) Furthermore, one might then expect that the simple trial wave function would be a better estimate of the solution to the altered problem because of the zero rate of change of the potential in the core region. Because our minimum of $+8.15$ Mev is already about 17 Mev above the experimental value, it is extremely likely that the exact solution to the altered problem is also higher than the experimental value. If this is true, the complete Gartenhaus potential must lead to a triton ground-state energy which is even higher. If E_{ex} , E , and E' are, respectively, the measured triton energy, the exact energy predicted by the Gartenhaus potential, and the exact energy predicted by the coreless Gartenhaus potential, the inequality

$$E_{\text{ex}} < E' < E, \quad (6)$$

would seem to hold by virtue of the calculated inequality

$$E_{\text{ex}} \ll E_V' < E_V. \quad (7)$$

In the latter the subscript V refers to the estimate obtained from the variational calculation.

III. DISCUSSION

A comparison of the matrix elements of H for the deuteron and triton indicates that the tensor potential is much more effective in binding the former than the latter. The interference term between the S and D states, brought about by the even-parity tensor potential, is critical for the binding of both nuclei and

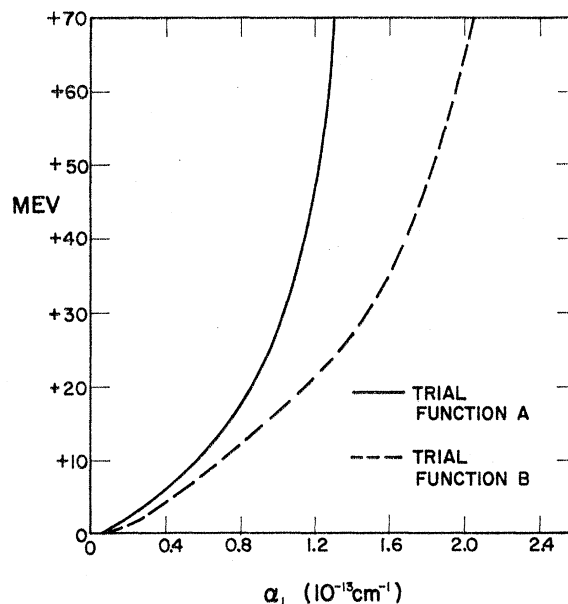


FIG. 1. Total energy as a function of α_1 along the curve $\partial E(\alpha_1, \alpha_7)/\partial \alpha_7 = 0$.

only in the deuteron is it sufficiently large. This can be clearly seen in Table I.

The relative ineffectiveness of the tensor potential in lowering the energy of the three-body system has long been known. Avery and Adams¹⁵ found that purely central potentials without repulsive cores yield binding energies for the triton and He^4 which are much too large; the addition of a tensor potential is necessary to make the total energy less negative. Pease and Feshbach¹⁶ used elaborate trial wave functions with a family of potentials, each member of which gave a good fit to the low-energy two-nucleon experimental data. They showed that the higher the deuteron D -state admixture a given potential produces the smaller is the binding energy of the triton. The 6.9% deuteron D -state admixture of the Gartenhaus potential should be compared to the 3.6% of the potential with which Pease and Feshbach obtained estimates of the triton binding energy which were too small.

Our results suggest, then, that the Gartenhaus potential is unsuitable for the three-body nuclear system because its even-parity central potentials are too weakly attractive compared to the even-parity tensor potential. A large tensor component appears in derivations of nucleon forces from meson theory and this property is already present in the one-meson exchange contribution to the nucleon-nucleon force. A large number of workers¹ take the nucleon-nucleon potential to be reliably given by meson theory for $r \geq 1/\mu$ but, unlike Gartenhaus, construct the potential in the inner regions phenomenologically so as to give a

¹⁵ R. Avery and E. N. Adams, Phys. Rev. 75, 1106 (1949).

¹⁶ R. L. Pease and H. Feshbach, Phys. Rev. 88, 945 (1952).

TABLE I. A comparison of the matrix elements of the deuteron and triton at minimum energy. For this comparison the strengths of the cores in the Gartenhaus potential have been set equal to zero. Only the principal triton D state has been used.

Matrix element	Deuteron (Mev)	Triton (Mev)
$\langle S H S\rangle$	+21.74	+15.957
$\langle S H D\rangle$	-78.12	-36.479
$\langle D H D\rangle$	+224.4	+179.38
E total	-4.83	+8.1843

fit to low- and high-energy data. In most cases D -state admixtures to the deuteron of the order of 7% are predicted from these potentials. This is consistent with the work of Biedenharn, Blatt, and Kalos¹⁷ who have shown that for triplet even-parity potentials with weak central parts, the admixture of D state increases rapidly with increasing hard-core radius. (In general, one is forced to choose fairly large hard-core radius in order to obtain a fit to high-energy scattering data.) If it is true that the Gartenhaus potential fails to bind the triton because of its very strong tensor force and large radius repulsive core, one can perhaps conclude that the nucleon-nucleon force must be taken to be strongly energy dependent in its inner region if in the outer region the force derived from meson theory is to be used.

It should be pointed out that we have included only one of the three linearly independent D states in our trial wave function. Hu and Hsu¹⁸ have shown that the presence of all three is necessary, if one is to obtain an accurate estimate of the ground-state energy since the two-body tensor operator acting on any one of the D states produces a linear combination of all three. We have made an estimate of the effect of adding the other two D states and found that their presence can lower the energy by about 4 Mev. One of the additional D states, $\Psi_6^{m,t}$, has the following form:

$$\Psi_6^{m,t} = \{ [(\boldsymbol{\rho} \cdot \mathbf{r})\eta^t - (\rho^2 - 3r^2)\eta^t][(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\rho})(\boldsymbol{\sigma}_3 \cdot \boldsymbol{\rho}) + 3(\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_3 \cdot \mathbf{r}) - \frac{1}{3}(\rho^2 + 3r^2)(\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_3)] \} \times \varphi^m f_6(\alpha_6, r_{ij}). \quad (8)$$

Noting that it is quartic in the position coordinates, it is clear that its various terms have more nodal surfaces in the space of the relative coordinates than do the terms in $\Psi_7^{m,t}$. Therefore, one would expect the following inequalities to hold:

$$\begin{aligned} & |\langle \Psi_1 | V_{T^+} | \Psi_6 \rangle| / |\langle \Psi_1 | V_{T^+} | \Psi_7 \rangle| = g_6 < 1, \\ & |\langle \Psi_6 | H | \Psi_6 \rangle| / |\langle \Psi_7 | H | \Psi_7 \rangle| \\ & \cong |\langle \Psi_6 | \text{K.E.} | \Psi_6 \rangle| / |\langle \Psi_7 | \text{K.E.} | \Psi_7 \rangle| = h_6 > 1. \end{aligned} \quad (9)$$

We have evaluated the above ratios for the easily

¹⁷ L. C. Biedenharn, J. M. Blatt, and M. H. Kalos, Nuclear Phys. **6**, 359 (1958).

¹⁸ T. Hu and K. Hsu, Proc. Roy. Soc. (London) **A204**, 476 (1950).

computed special case of

$$\begin{aligned} f_i &= \exp[-\alpha_i(r+P)], \\ V_{T^+}(12) &= V_T \exp(-\gamma r_{12}), \\ 1/\gamma &= 1.4 \times 10^{-13} \text{ cm.} \end{aligned} \quad (10)$$

The α_i 's were chosen such that each α_i led to a value of $\langle \Psi_i | e^2/r_{12} | \Psi_i \rangle$ which was equal to the $\text{H}^3\text{-He}^3$ energy difference. The values obtained for g_6 and h_6 are $g_6=0.63$ and $h_6=1.28$. Assuming that these ratios are approximately true independently of the potential and also hold roughly for the third D state, $\Psi_8^{m,t}$, one can evaluate a new triton energy as a function of

$$\sum_{i=6}^8 |A_i|^2 = D^2.$$

In the latter expression D^2 is the total D -state probability and A_i is the amplitude of the i th D state. Table II below shows a sizable decrease in the energy but one which is not nearly large enough to remove the discrepancy.

The only other state coupled directly to the principal S state which has been omitted is the partially space antisymmetric S state

$$\Psi_2^{m,t} = \{ (\mathbf{r} \cdot \boldsymbol{\rho})(12\varphi^m\eta^t - \bar{\varphi}^m\bar{\eta}^t) - (\rho^2 - 3r^2)(\varphi^m\bar{\eta}^t + \bar{\varphi}^m\eta^t) \} f_2(\alpha_2, r_{ij}).$$

It is coupled to Ψ_1 by the combination of potentials ${}^1V_{C^+}(12) - {}^3V_{C^+}(12)$. In the core region this quantity can be of the order of -100 Mev but goes to zero more rapidly with increasing r_{12} than either potential separately. This is due to the fact that to second order in the meson coupling constant the two potentials must be equal in a charge symmetric theory and for sufficiently large r_{12} the second-order terms dominate. For example, at $r_{12}=2.0 \times 10^{-13}$ cm, ${}^1V_{C^+} = -5$ Mev, ${}^3V_{C^+} = -3$ Mev, and $V_{T^+} = -10$ Mev. From the above numbers one can see that at distances comparable to the average internucleon separation,^{5,19}

$$\langle (r_{ij}^2)_{\text{av}} \rangle = (3\langle r^2 \rangle_{\text{rms}})^{1/2} \cong 2.5 \times 10^{-13} \text{ cm,}$$

the coupling of Ψ_2 to Ψ_1 is weak compared to the coupling of the D states to Ψ_1 .

TABLE II. Change in total energy of the triton as a function of total D -state probability with all three linearly independent D states present. In this estimate $\langle \Psi_6 | V_T | \Psi_{6,8} \rangle$ has been taken to be equal to 0.63 $\langle \Psi_1 | V_T | \Psi_7 \rangle$ and $\langle \Psi_{6,8} | H | \Psi_{6,8} \rangle$ equal to 1.28 $\langle \Psi_7 | H | \Psi_7 \rangle$. The values of the necessary matrix elements have been taken from Table I.

D^2	$A_6^2 = A_8^2$	A_7^2	E (Mev)
4.6%	0	4.6%	+8.2
5%	0.77%	3.47%	+3.8
6%	0.86%	4.28%	+3.6
7%	0.97%	5.07%	+3.9

¹⁹ C. Wernitz, Nuclear Phys. **16**, 59 (1960).

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APPENDIX

The requirement that the energy be a minimum with respect to the coefficients A_1 and A_7 [Eq. (1-a)] yields the secular equation for $E(\alpha_1, \alpha_7)$ in terms of the matrix elements of the Hamiltonian H :

$$\begin{vmatrix} E(\alpha_1, \alpha_7) - \langle \Psi_1 | H | \Psi_1 \rangle & \text{Re} \langle \Psi_7 | H | \Psi_1 \rangle \\ \text{Re} \langle \Psi_1 | H | \Psi_7 \rangle & E(\alpha_1, \alpha_7) - \langle \Psi_7 | H | \Psi_7 \rangle \end{vmatrix} = 0. \quad (\text{A-1})$$

Because of the complete antisymmetry of the trial functions the Hamiltonian for the inner motion of the triton is equivalent to

$$H = -(\hbar^2/M)[3\nabla_{12} \cdot \nabla_{12} - 3\nabla_{12} \cdot \nabla_{23}] + 3[V_C^+(r_{12}) + {}^1V_C^-(r_{12}) + {}^3V_C^+(r_{12}) + {}^3V_C^-(r_{12})] + 3[V_T^+(r_{12}) + V_T^-(r_{12})]S_{12}. \quad (\text{A-2})$$

In the above, ∇_{ij} refers to the gradient with respect to r_{ij} , S_{12} is the usual tensor operator, and the four V_C 's and two V_T 's constitute the spin- and parity-dependent Gartenhaus potential. The projection operators which usually precede each component of the potential have been omitted because the structure of Ψ_1 and Ψ_7 with respect to the pair 1,2 makes their explicit use unnecessary. It should be pointed out that the above form of the kinetic energy operator requires one to consider r_{13} to be independent of r_{12} and r_{23} . That is to say, $\nabla_{12}r_{13} = \nabla_{23}r_{13} = 0$.

Using the definitions of Ψ_1 and Ψ_7 given in Eq. (1), the kinetic energy and potential energy matrix elements have the following form after being summed over spin and isotopic spin:

$$\begin{aligned} (\text{a}) \quad & \langle \Psi_1 | \text{K.E.} | \Psi_1 \rangle = +24(\hbar^2/M)N_1^{-1}[3\langle \nabla_{12}f_1(\alpha_1, r_{ij}) \cdot \nabla_{12}f_1(\alpha_1, r_{ij}) \rangle - 3\langle \nabla_{12}f_1(\alpha_1, r_{ij}) \cdot \nabla_{23}f_1(\alpha_1, r_{ij}) \rangle], \\ (\text{b}) \quad & \langle \Psi_1 | V | \Psi_1 \rangle = 36N_1^{-1}\langle f_1(\alpha_1, r_{ij}) | {}^1V_C^+(r) + {}^3V_C^+(r) | f_1(\alpha_1, r_{ij}) \rangle, \\ (\text{c}) \quad & \text{Re} \langle \Psi_1 | V_T | \Psi_7 \rangle = 24(N_1N_7)^{-1/2}\langle f_1(\alpha_1, r_{ij}) | [\rho^2 - 3(\mathbf{p} \cdot \mathbf{r})/r^2 + 6r^2] {}^3V_T^+(r) | f_7(\alpha_7, r_{ij}) \rangle, \\ (\text{d}) \quad & \langle \Psi_7 | \text{K.E.} | \Psi_7 \rangle = +8(\hbar^2/M)N_7^{-1}\{ \langle f_7(\alpha_7, r_{ij}) | 30\rho^2 + 90r^2 | f_7(\alpha_7, r_{ij}) \rangle + \langle \nabla_{12}f_7(\alpha_7, r_{ij}) \cdot \nabla_{12}f_7(\alpha_7, r_{ij}) \rangle \\ & + \mathbf{r}(24\rho^2 + 6\mathbf{p} \cdot \mathbf{r} + 36r^2) | f_7(\alpha_7, r_{ij}) \rangle + \langle \nabla_{23}f_7(\alpha_7, r_{ij}) \cdot \nabla_{23}f_7(\alpha_7, r_{ij}) \rangle + \langle \mathbf{p}(6\mathbf{p} \cdot \mathbf{r}) - \mathbf{r}(12\rho^2 + 18r^2) | f_7(\alpha_7, r_{ij}) \rangle \\ & + \langle \nabla_{12}f_7(\alpha_7, r_{ij}) \cdot \nabla_{12}f_7(\alpha_7, r_{ij}) \rangle + \langle \nabla_{23}f_7(\alpha_7, r_{ij}) \cdot \nabla_{23}f_7(\alpha_7, r_{ij}) \rangle \\ & + \langle \nabla_{12}f_7(\alpha_7, r_{ij}) \cdot \nabla_{23}f_7(\alpha_7, r_{ij}) \rangle \}, \\ (\text{e}) \quad & \langle \Psi_7 | V | \Psi_7 \rangle = 8N_7^{-1}\langle f_7(\alpha_7, r_{ij}) | {}^3V_C^-(r)[9\rho^2r^2 + 3(\mathbf{p} \cdot \mathbf{r})^2] + {}^3V_C^+(r)[\rho^4 + 3\rho^2r^2 + 9r^4 - 9(\mathbf{p} \cdot \mathbf{r})^2] + {}^3V_T^-(r) \\ & \times [-9\rho^2r^2 - 15(\mathbf{p} \cdot \mathbf{r})^2] + {}^3V_T^+(r)[\rho^4 - 6\rho^2r^2 - 18r^4 + 18(\mathbf{p} \cdot \mathbf{r}) - 3(\mathbf{p} \cdot \mathbf{r})^2\rho^2/r^2] | f_7(\alpha_7, r_{ij}) \rangle. \end{aligned} \quad (\text{A-3})$$

The normalization constants are defined by

$$\begin{aligned} (\text{a}) \quad & N_1 = 24\langle f_2(\alpha_1, r_{ij}) | f_1(\alpha_1, r_{ij}) \rangle, \\ (\text{b}) \quad & N_7 = \langle f_7(\alpha_7, r_{ij}) | (8/3)\rho^4 + 32\rho^2r^2 + 24r^4 \\ & - 16(\mathbf{p} \cdot \mathbf{r})^2 | f_7(\alpha_7, r_{ij}) \rangle. \end{aligned} \quad (\text{A-4})$$

After inserting the appropriate forms for f_1 and f_7 , the integrations were performed by making the change of variables

$$\begin{aligned} s &= (r_{23} + r_{13})/2, \quad t = (r_{23} - r_{13})/2, \\ r_{12} &= r_{12}. \end{aligned} \quad (\text{A-5})$$

As a result, the integral

$$\begin{aligned} & \int_0^\infty dr_{12} \int_0^{r_{12}} dr_{23} \int_{r_{12}-r_{23}}^{r_{12}+r_{23}} dr_{13} (r_{12}r_{23}r_{13}) F(r_{12}, r_{23}, r_{13}) \\ & + \int_0^\infty dr_{12} \int_{r_{12}}^\infty dr_{23} \int_{r_{23}-r_{12}}^{r_{12}+r_{23}} dr_{13} (r_{12}r_{23}r_{13}) \\ & \times F(r_{12}, r_{23}, r_{13}) \end{aligned} \quad (\text{A-6})$$

is changed to

$$\frac{1}{4} \int_0^\infty dr_{12} \int_{r_{12}}^\infty ds \int_{-r_{12}}^{+r_{12}} dt r_{12}(s^2 - t^2) F(r_{12}, s, t).$$

This transformation permitted the reduction of the potential energy elements to single-fold integrals over r_{12} which were performed numerically. The integrals are too unwieldy to be listed here.