tritium, He^3, and α-particles. To build across the mass 5 and 8 gaps, it is necessary to assume triple collisions such as α—n—n and α—α—n and processes such as $Li^7(\alpha, n)B^{10}$. Difficulties of another type arise at masses 10 and 14. Be^{10} and C^{14} both have half-lives of more than 1000 years while Be^{11} and C^{15} are probably neutron unstable. From $A=15$ on, there seem to be no breaks in the formation chain due to nuclear instability or long-lived β-emitters which cannot be bypassed.

The formation of the elements then appears to be divided into two distinct parts. For $A>16$, the process is essentially one of building heavy nuclei by successive neutron captures interspersed by β-decays. In this region, there are two other reactions which are of some importance to the formation process. They are the nuclear photo-effect, which may be responsible for the creation of isobars,[6] and fission in the heaviest elements, which sets an upper limit on the size of nuclei formed. For $A<16$, there are many types of reactions having probabilities of the order of magnitude of the neutron capture probability, and any attempt to compute the relative abundances of light elements must consider all of them.

VI. ACKNOWLEDGMENTS

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Tensor Forces and the Triton Binding Energy*

Herman Feshbach
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts

and

William Rarita**
Physics Department, Brooklyn College, Brooklyn, New York

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The binding energy of the triton has been calculated variationally employing the Hylleraas expansion for the trial wave functions, thus permitting a systematic improvement in the binding energy. The procedure used was tested by applying it to the binding energy problem of the deuteron with tensor forces. The present theory, assuming a rectangular-well shape with a range of 2.8×10^{-13} cm for all the internucleon potentials, yields a H^3 binding energy 40 percent to 50 percent of the experimental value. Various suggestions for resolving this dilemma are discussed.

I. INTRODUCTION

The explanation of the properties of the triton is a severe test of the phenomenological theory of nuclear forces. Prior to the introduction of tensor forces, its calculated[1] binding energy was in good agreement with experiment. It was realized at an early date by Inglis[2] that this situation might be substantially altered when tensor forces are included in spite of the rather complete explanation of two-body problems[3] afforded by the Rarita-Schwinger theory. In the H^3 problem, their interaction potential, a rectangular well, is tested for larger relative momenta of the constituent nucleons. Inglis' argument was based on perturbation theory. A more complete discussion has been given by Gerjuoy and Schwinger,[4] using the variational method with results in substantial agreement with Inglis. It is the aim of the present paper to enlarge the scope of the former's work by the use of the method of Hylleraas which has been applied successfully to problems of this type in the past.[1] We shall use the two-body law of force as given by Rarita and Schwinger.[5] Their results do not determine the exchange character of the nuclear force but this property does not enter crucially into our discussions. The main conclusion of the present paper is that the simple theory which works so well

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** This work was done while the second author (W.R.) was in residence at Massachusetts Institute of Technology. He takes this opportunity to express his appreciation for the hospitality shown him during his stay there.

[1] W. Rarita and R. D. Present, Phys. Rev. **51**, 788 (1937).

[2] David R. Inglis, Phys. Rev. **55**, 988 (1939).

[3] See for example: Bailey, Bennet, Bergstralh, Nuckolls, Richards, and Williams, Phys. Rev. **70**, 583 (1946). Russell, Sachs, Wattenberg, and Field, Phys. Rev. **73**, 545 (1948). R. Wilson, C. H. Collie, and H. Halban, Nature **162**, 185 (1948).

[4] E. Gerjuoy and J. Schwinger, Phys. Rev. **61**, 138 (1941).

[5] W. Rarita and J. Schwinger, Phys. Rev. **59**, 436 and 556 (1941).

for two-body problems fails for H^3. We shall discuss some possible modifications in the concluding section.

II. TRITON BINDING ENERGY

We shall employ the relative coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, $\boldsymbol{\rho}$ illustrated in Fig. 1. After the coordinates of the center of mass are eliminated the Hamiltonian for this problem may be expressed in terms of these coordinates:

$$H=-(\hbar^2/M)(\nabla_1^2+\nabla_1\cdot\nabla_2+\nabla_2^2)+V(r_1)+V(r_2)+V(\rho). \quad (1)$$

The potential energy V is

$$V(\rho)=-\{1-\tfrac{1}{2}g+\tfrac{1}{2}g\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2+\gamma S_{12}\}J(\rho). \quad (2)$$

Here $\boldsymbol{\sigma}_i$ is the Pauli spin vector associated with the ith particle, and

$$S_{12}=[3(\boldsymbol{\sigma}_1\cdot\boldsymbol{\rho})(\boldsymbol{\sigma}_2\cdot\boldsymbol{\rho})/\rho^2]-\sigma_1\cdot\sigma_2. \quad (3)$$

$V(r_1)$, the potential between particles 1 and 3 is obtained by replacing $\boldsymbol{\sigma}_2$ by $\boldsymbol{\sigma}_3$ in (2) and (3) and $\boldsymbol{\rho}$ by $\mathbf{r}_1$. The constants g and γ, are given by Rarita and Schwinger[5] for a rectangular potential well of depth V_0 and range r_0:

$$\begin{aligned}&g=0.0715,\quad \gamma=0.775,\\&V_0=6.40\times\text{binding energy of the deuteron},\\&r_0=2.80\cdot 10^{-13}\text{ cm}.\end{aligned} \quad (4)$$

The ground state of H^3 has a total angular momentum of $\frac{1}{2}\hbar$. For a three-particle system the possible orbital angular momentum states are S, P, D. The S states must be doublets, the D states quartets, while the P states may be either doublet or quartets. The angular and spin dependence may be removed either in terms of the Eulerian angles associated with the plane containing the three particles[6] or much more conveniently by the use of spin operators as performed by Gerjuoy and Schwinger. From the measured magnetic moment[7] of H^3, it may be seen that the principal state is an S state. Of the two S states which can be formed, the most important will be that one symmetric in r_1 and r_2; its angular and spin dependence will be represented by ${}^2S_{\frac{1}{2}}{}^0$; the other S state ${}^2S_{\frac{1}{2}}{}^1$ will be antisymmetric in r_1 and r_2. In virtue of Hamiltonian the ${}^2S_{\frac{1}{2}}{}^0$ state will interact directly with the ${}^2S_{\frac{1}{2}}{}^1$ state and with the ${}^4D_{\frac{1}{2}}$ states. These latter may be formed as shown by Gerjuoy and Schwinger from the four operators which may be realized by combining the dyadic $\boldsymbol{\sigma}_1\boldsymbol{\sigma}_3$ with the space dyadics $\mathbf{r}_1\mathbf{r}_1$, $\mathbf{r}_1\mathbf{r}_2$, etc. However, it has been shown by L. H. Thomas[8] that an identity exists between these four so that there are only three independent D states, which we shall call ${}^4D_{\frac{1}{2}}{}^0$, ${}^4D_{\frac{1}{2}}{}^1$, ${}^4D_{\frac{1}{2}}{}^2$. This may be verified directly using the more explicit Eulerian angular dependence.[9] Only one of these D states has a dependence on r_1 and r_2 which is even in their exchange:

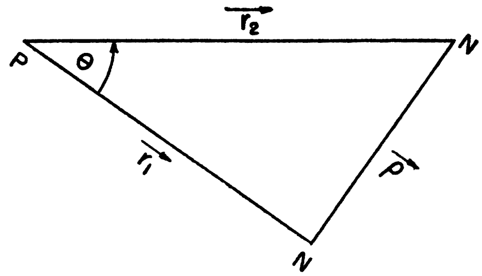

FIG. 1. Coordinates for H^3.

$${}^4D_{\frac{1}{2}}{}^0=(r_1{}^2S_{13}+r_2{}^2S_{23})\,{}^2S_{\frac{1}{2}}{}^0. \quad (5)$$

It will be assumed here as in Gerjuoy and Schwinger that this state is the principal one combining with the ground state ${}^2S_{\frac{1}{2}}{}^0$. The qualitative argument upon which this is based relies on the fact that the ${}^4D_{\frac{1}{2}}{}^{1,2}$ states are odd in the exchange of r_1 and r_2 and thus must have a node whenever $r_1=r_2$, i.e., whenever the two neutrons are close together. From the short range character of the forces it follows that $V(\rho)$ will have relatively little average value for these states. A similar argument may be applied to the ${}^2S_{\frac{1}{2}}{}^1$ state which is known to be present in a relatively small amount in the ground state of H^3.

We therefore write for the wave-function Ψ:

$$\Psi=f\,{}^2S_{\frac{1}{2}}{}^0+g\,{}^4D_{\frac{1}{2}}{}^0, \quad (6)$$

where f and g will depend only upon r_1, r_2, and ρ. Finally

$${}^2S_{\frac{1}{2}}{}^0=(1/8\pi)^{\frac{1}{2}}\alpha(3)[\alpha(1)\beta(2)-\beta(1)\alpha(2)], \quad (7)$$

where α and β are the usual spin functions. Expression (6) may now be introduced into the variational principal to obtain the energy E:

$$E=(\Psi, H\Psi)/(\Psi, \Psi). \quad (8)$$

The explicit expressions are given in the Appendix.

The functions f and g were determined by the method of Hylleraas. The functional forms assumed first were

$$\begin{aligned}f&=A\exp[-\lambda(r_1+r_2)-\nu\rho],\\g&=B\exp[-\mu(r_1+r_2)-\sigma\rho].\end{aligned} \quad (9)$$

When a variational function of the type f is used in the Rarita-Present theory, one obtains immediately 90 percent of the binding energy of H^3, which indicates that it is an excellent description of the S state. Once the proper values of λ, μ, ν, σ are determined both f and g are to be multiplied

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[6] E. C. Kemble, *The Fundamental Principles of Quantum Mechanics* (McGraw-Hill Cook Company, Inc., New York, 1937), p. 230.

[7] H. Anderson and A. Novick, Phys. Rev. **71**, 372 (1947).

[8] Private communication.

[9] Herman Feshbach, Phys. Rev. **61**, 544A (1942).

TABLE I. Percent experimental binding energy.

Nucleus	S state (no tensor forces)	S and D	S	D
H^2	74	66	−46	112
H^3	70	32	18	14
H^3			28 Equivalent Two Body	

by power series in r_1, r_2, and ρ. For variational functions (9) it was found that $\lambda \simeq \nu$ and $\sigma \sim 0$ although equalities did not occur precisely at the minimum. However, because the difference in binding energy involved was slight (about 3 percent) the simpler expressions obtained by assuming equality were used with

$$\lambda = \nu = 1.5/r_0; \quad \sigma = 0; \quad \mu = 5.0/r_0. \tag{10}$$

The binding energy found using function (10) was 32 percent of the experimental binding energy, and the percent D state = 1.7 percent.

The next step involved the use of the Hylleraas expansion for both f and g. In the present calculation terms up to the squares of r_1+r_2, and ρ and their crossproducts were included. Thus ten more terms, five for the S state and five for the D state were considered. *No marked improvement in the binding energy was obtained when the coefficients of these terms were varied, indicating that form (9) was already a good approximation to the correct wave functions.* The final value for the calculated H^3 binding energy was 40 percent of the experimental value.

To buttress this conclusion, we have checked upon our results by comparing with similar calculations for the deuteron and by employing the equivalent two body[10] method to estimate the contribution of the S state to the total energy. These results, are summarized in Table I.

We have given our results for the case of the simple function (10). For the more complicated Hylleraas expansion, we estimate that the entries in columns (3) and (4) for H^3 would change to 21 and 19, respectively.

The first column S gives the energy computed using the potential energy required to obtain the binding energy of H^2 before the discovery of the deuteron quadrupole moment, and thus in the absence of tensor forces. The second column yields the total energy when potential energy (2) is used. The decomposition in the third and fourth columns gives the energy obtained from the S state alone and the energy obtained from the D state together with the coupling energy between the S and D states.

We first note that the equivalent two body method gives for the binding energy from the S state alone, the value 28 percent of the experimental binding energy of H^3. This value is to be compared with 18 percent for the trial function (10) and 21 percent for the Hylleraas expansion, remembering that the two body method may give a value 10 to 15 percent too large in absolute value. The rough agreement obtained indicates that our representation of the S state is excellent. No such check is available for the D state energy so that we must rely on the indirect evidence offered by the above S state comparison, and the data in the table. Here we see that for the simplest variational form used for H^2 the energies computed with and without tensor forces are very close. Moreover when a power series expansion was added on to the deuteron wave functions the rate of improvement was similar to that obtained for H^3 with the Hylleraas expansion. We would like to emphasize the drastic change in the comparison between the computed energies for the binding energy of H^3 with and without tensor forces. Moreover the decomposition in S and D energy given in columns (3) and (4) lends additional weight that no gross inaccuracy can be ascribed to our final values.***

As a final check, the contribution of the ${}^2S_{\frac{1}{2}}{}^1$ state was computed using form (10) for the ${}^2S_{\frac{1}{2}}{}^0$ and ${}^2D_{\frac{1}{2}}{}^0$ terms. The ${}^2S_{\frac{1}{2}}{}^1$ state couples directly to the ${}^2S_{\frac{1}{2}}{}^0$ state. It is fairly representative of the many omitted states noted above. We then let

$$\Psi = f\,{}^2S_{\frac{1}{2}}{}^0 + g\,{}^4D_{\frac{1}{2}}{}^0 + h\,{}^2S_{\frac{1}{2}}{}^1. \tag{11}$$

The function h must be odd in exchange of r_1 and r_2 so that as in Rarita and Present h must be taken proportional to r_1-r_2. Then

$$h = D(r_1-r_2)\exp[-\alpha(r_1+r_2+\rho)],$$

where D and α are to be determined variationally. The resulting increase in binding energy is only 0.4 percent indicating that these additional terms will not affect the binding energy of H^3 to any great extent. We thus conclude that the computed binding energy of H^3 employing nuclear potentials (2) and (4) is not appreciably greater than 40 percent of the experimental value.

III. DISCUSSION

It is appropriate now to discuss some of the possible changes in the internucleon potentials which might bring the theoretical value for the binding energy of H^3 into agreement with experiment. One might hope to resolve the difficulty by (1) keeping the Rarita-Schwinger potential intact

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[10] Eugene Feenberg, Phys. Rev. **47**, 850 (1935); **48**, 906 (1935).

*** One of us (W.R.) has used a joining method (described Phys. Rev. **74**, 1799 (1948)), to compute the binding energy. Here f and g are assumed to have different radial dependence inside and outside of an arbitrary radius. The best binding thus obtained was 36 percent.

and adding forces which are of some importance in H^3 and of relatively little importance in H^2, and (2) changing the shape and range of the interaction potential.

Considering method (1) first, a measure of the additional potential required is given by the ratio τ of the V_0 needed to the V_0 used in (4). We estimate $\tau \sim 1.1$. Such additional potentials can in principle arise from relativistic effects since v^2/c^2 of a nucleon in H^3 is appreciable. Relativistic effects include three body forces[11] beside relativistic corrections[12] to two body forces. The latter will probably be made available as a result of experiments on high energy neutron-proton scattering. It should be noted however that such additional potentials as contemplated above would not correct other difficulties of the Rarita-Schwinger interaction potential.[13]

In category (2) we have investigated briefly the effects of a change in range, or shape, or both, of the interaction potential. *Decreasing* the range of *both* the central and tensor forces *decreases* the calculated binding energy of H^3. For example using the range[14] $2.66 \cdot 10^{-13}$ cm with a rectangular well potential for $J(r)$, the calculated binding energy of H^3 decreases to 24 percent of the experimental value for the same trial functions which yield 32 percent. The qualitative reason for this behavior may be given. Reducing the range requires a greater relative amount of tensor force, i.e., a greater γ, for only in this way is it possible to obtain the experimental quadrupole moment for the deuteron. However a large γ requires a smaller V_0 (in order to obtain the experimental binding energy of the deuteron), leading to a reduction in the calculated binding energy of H^3. Since present two body data requires, if anything, a reduction in range, changing the range of both central and tensor forces does not seem to be a fruitful idea.

Another possibility then would involve maintaining the range of the central force to that given by p–p scattering data, but using a longer range tensor force. Primakoff and Feenberg[15] have pointed out that by taking the tensor range sufficiently long the tensor force would have no effect on binding energy problems, so that the binding energy problem would return to the pre-tensor situation. Here however a difficulty encountered by Rarita and Present would recur, for although H^3 binding would be precisely correct, the calculated binding energy for He^4 would be too large. This has been verified for other potential wells by Svartholm.[16] It is essential, therefore that the tensor force be of sufficient strength as to effect the binding of H^2 considerably, of H^3 somewhat, and of He^4 not at all. This adjustment is very sensitive to the *shape* of the interaction potential.†

Finally one might give up the luxury of charge independent nuclear forces as suggested by Blatt.[13] It would be necessary to keep the (n–n) and (p–p) forces the same because of evidence obtained from the energy differences of mirror nuclei, particularly the H^3-He^3 binding energy difference. It is, however, possible to reduce the range of either the singlet n–p force or the central (non-tensor) part of the triplet (n–p) force. It should be noted that such an interaction potential would in addition yield results closer to the present scattering data than the Rarita-Schwinger ansatz.

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We are indebted to Miss Hannah Paul for computational aid.

APPENDIX

Variational Calculation for the Deuteron

The deuteron serves as a useful introduction and control to the more difficult triton problem. The energy E of the deuteron ground state is

$$\begin{aligned} &E\int_0^\infty [(Au)^2+(Bw)^2]dr \\ &=\int_0^\infty \{[d(Au)/dr]^2-JA^2u^2-4\sqrt{2}\gamma JABuw \\ &\qquad -(1-2\gamma)JB^2w^2+(6B^2w^2/r^2)+[d(Bw)/dr]^2\}dr. \end{aligned} \tag{A1}$$

Here Au/r is the S radial wave function and Bw/r is the D radial function. Varying the coefficients leads to a secular equation

$$\|E_{ij}\|=0,\quad E_{ij}=P_{ij}-L_{ij}-EN_{ij}. \tag{A2}$$

Using the binding energy of the deuteron $|E_0|$ as the unit of energy:

$$\begin{aligned} &P_{11}=1/\alpha^2\int_0^\infty (du/dr)^2dr,\quad \alpha^2=M|E_0|/\hbar^2, \\ &P_{12}=0, \\ &P_{22}=1/\alpha^2\int_0^\infty [(dw/dr)^2+6(w^2/r^2)]dr, && N_{11}=\int_0^\infty u^2dr, \\ &L_{11}=\int_0^\infty Ju^2dr, && N_{12}=0, \\ &L_{12}=2^{\frac{3}{2}}\int_0^\infty \gamma Juwdr, && N_{22}=\int_0^\infty w^2dr, \\ &L_{22}=\int_0^\infty (1-2\gamma)Jw^2dr. \end{aligned} \tag{A3}$$

Let J be the rectangular well. Use r_0, its range, as the unit of distance. Let $u=re^{-\lambda r}$, $w=r^3e^{-\mu r}$. All the integrals are easily

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[11] H. Primakoff and T. Holstein, Phys. Rev. **55**, 1218 (1939).

[12] Gregory Breit, Phys. Rev. **56**, 153 (1938).

[13] D. Bohm and C. Richman, Phys. Rev. **21**, 567 (1947); J. Blatt, Phys. Rev. **74**, 92 (1948).

[14] William G. Guindon, S.J., Phys. Rev. **74**, 145 (1948).

[15] Henry Primakoff, Phys. Rev. **72**, 118 (1947).

[16] N. Svartholm, Thesis.

† Since the calculations reported here were completed, one of us (H.F.) has shown that a potential

$$\begin{gathered} V(\rho)=-[(1-\tfrac{1}{2}g)+\tfrac{1}{2}g\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2]V_c(\rho)+S_{12}V_\tau(\rho) \\ V_c=V_{0c}(e^{-\mu\rho}/\mu\rho)\quad V_\tau=V_{0\tau}(e^{-\tau\rho}/\tau\rho) \\ \mu=326\ \mathrm{mc}/\hbar\quad \tau=\mu/1.8 \end{gathered}$$

yields on a variational calculation 85.5 percent of the experimental H^3 binding.

evaluated. The integrals involved are of the form

$$\int_0^1 r^n e^{-\nu r} dr = I_n^\nu, \quad \int_0^\infty r^n e^{-\nu r} dr = S_n^\nu. \tag{A4}$$

Variational Calculation for H^3

We list the elements of the matrices P_{ij}, L_{ij}, N_{ij}. The determinant is, of course, of the form (A2). The elements P_{11}, L_{11}, and N_{11} listed first are well known being given in Rarita and Present.

$$P_{11} = \int \left\{ \left(\frac{\partial f}{\partial r_1}\right)^2 + \left(\frac{\partial f}{\partial r_2}\right)^2 + \left(\frac{\partial f}{\partial \rho}\right)^2 + \frac{\mathbf{r}_1 \cdot \mathbf{r}_2}{r_1 r_2} \frac{\partial f}{\partial r_1} \frac{\partial f_2}{\partial r_2} + \frac{\mathbf{r}_1 \cdot \mathbf{r}_{21}}{r_1 \rho} \frac{\partial f}{\partial r_1} \frac{\partial f}{\partial \rho} + \frac{\mathbf{r}_2 \cdot \mathbf{r}_{12}}{r_2 \rho} \frac{\partial f}{\partial r_2} \frac{\partial f}{\partial \rho} \right\} d\tau;$$
$$d\tau = 4 r_1 r_2 \rho \, dr_1 dr_2 d\rho. \tag{A5}$$

$$L_{11} = (1-2g) L^S(12) + (1-g/2)[L^S(13) + L^S(23)],$$

$$L^S(12) = \int f^2 J(\rho) d\tau, \quad L^S(13) + L^S(23) = \int f^2 [J(r_1) + J(r_2)] d\tau.$$

The coupling term E_{12} is:

$$\begin{aligned} E_{12} &= -2\gamma \int f\, {}^2S_{\frac{1}{2}}^0 J(r_1) g\, {}^2D_{\frac{1}{2}}^0 d\tau \\ &= -2\gamma \int f J(r_1) g [6 r_1^2 + (3 - 9\cos^2\theta) r_2^2] d\tau. \end{aligned} \tag{A6}$$

The kinetic energy for the D state P_{22} is:

$$\begin{aligned} -P_{22} &= (g\, {}^4D_{\frac{1}{2}}^0 | \nabla_1^2 + \nabla_1 \cdot \nabla_2 + \nabla_2^2 | g\, {}^4D_{\frac{1}{2}}^0) \\ &= \int \left\{ \left[\frac{g}{r_1^2} \frac{\partial}{\partial r_1}\left(r_1^2 \frac{\partial g}{\partial r_1}\right) + \frac{g}{r_2^2} \frac{\partial}{\partial r_2}\left(r_2^2 \frac{\partial g}{\partial r_2}\right) + \frac{g}{\rho^2} \frac{\partial}{\partial \rho}\left(\rho^2 \frac{\partial g}{\partial \rho}\right) \right.\right. \\ &\quad + \frac{\mathbf{r}_1 \cdot \mathbf{r}_{21}}{r_1 \rho} g \frac{\partial^2 g}{\partial r_1 \partial \rho} + \frac{\mathbf{r}_2 \cdot \mathbf{r}_{12}}{r_2 \rho} g \frac{\partial^2 g}{\partial r_2 \partial \rho} \\ &\quad \left. + \frac{\mathbf{r}_1 \cdot \mathbf{r}_2}{r_1 r_2} g \frac{\partial^2 g}{\partial r_1 \partial r_2} + \frac{2}{\rho} g \frac{\partial g}{\partial \rho} \right] ({}^4D_{\frac{1}{2}}^0 / {}^4D_{\frac{1}{2}}^0) \\ &\quad + [6 r_1^4 + 3 r_1^2 r_2^2 (1 - 3\cos^2\theta)] \frac{4 g_1}{r_1} \frac{\partial g}{\partial r_1} \\ &\quad \left. + [6 r_2^4 + 3 r_1^2 r_2^2 (1 - 3\cos^2\theta)] \frac{4 g}{r_2} \frac{\partial g}{\partial r_2} \right\} d\tau, \end{aligned} \tag{A7}$$

where $({}^4D_{\frac{1}{2}}^0 | {}^4D_{\frac{1}{2}}^0) = 6[r_1^4 + r_2^4 + r_1^2 r_2^2 (1 - 3\cos^2\theta)]$.

$$\begin{aligned} L_{22} = [L^D(12) + L^D(13) + L^D(23)] \\ + \gamma [L_T^D(12) + L_T^D(13) + L_T^D(23)], \end{aligned} \tag{A8}$$

where the subscript T denotes tensor, the terms involved being diagonal values for the D state for the tensor terms.

$$\begin{aligned} L^D(12) &= \int g^2 J(\rho) d\tau; \quad L^D(13) = \int g^2 J(r_1) d\tau; \\ L^D(23) &= \int g^2 J(r_2) d\tau, \\ L_T^D(13) &= \int [6(r_2^4 - r_1^2 r_2^2 - 2 r_1^4) \\ &\quad - 3(1 - \cos^2\theta)(r_2^4 + r_1^2 r_2^2)] g^2 J(r_1) d\tau. \end{aligned} \tag{A9}$$

For $L_T^D(23)$ make substitutions $r_1 \rightleftarrows r_2$ in multiplication factor in square brackets and in $J(r_1)$.

$$\begin{aligned} L_T^D(12) = \int \Bigg\{ & 12\left[r_1^4 + r_2^4 + r_1^2 r_2^2 \left(\frac{3\cos^2\theta - 1}{2} \right) \right] \\ & - \frac{12}{\rho^2} [2 r_1^6 + 2 r_2^6 + (r_1^2 + r_2^2) r_1^2 r_2^2 \\ & - 3(r_1^4 + r_2^4) r_1 r_2 \cos\theta] \Bigg\} g^2 J(\rho) d\tau. \end{aligned} \tag{A10}$$

Finally

$$N_{22} = \int g^2 d\tau ({}^4D_{\frac{1}{2}}^0 / {}^4D_{\frac{1}{2}}^0). \tag{A11}$$

Assuming (10) for the D state and the rectangular well shape $N_{22} = (192)(6!)/\mu^{10}$; $P_{22} = (96)(6!)/\mu^8$;

$$\begin{aligned} L^D(12) &= +V_0 \left[\frac{8}{21} I_9^\mu + (S_4^\mu - I_4^\mu) - \frac{24}{35}(S_2^\mu - I_2^\mu) + \frac{1}{15}(S_0^\mu - I_0^\mu) \right]; \\ L^D(13) + L^D(23) &= +96 V_0 [S_6^\mu I_2^\mu + S_2^\mu I_6^\mu]; \\ L_T^D(12) &= V_0 \left\{ -\frac{32}{49} I_9^\mu - \frac{1}{3}(S_6^\mu - I_6^\mu) - (S_4^\mu - I_4^\mu) + \frac{183}{245}(S_2^\mu - I_2^\mu) - \frac{1}{15}(S_0^\mu - I_0^\mu) \right\}; \\ L_T^D(13) + L_T^D(23) &= +96 V_0 [+S_6^\mu I_2^\mu - S_4^\mu I_4^\mu - 2 S_2^\mu I_6^\mu]. \end{aligned} \tag{A12}$$

When the more complicated variational function (9) or the Hylleraas expansion are used more difficult integrals appear. Two auxiliary integrals had to be introduced.

$$\begin{aligned} H_{m,n}^{\alpha,\beta} &= \int_0^1 s^m e^{-\alpha s} ds \int_0^s \rho^n e^{-\beta\rho} d\rho, \\ G_{l,m,n}^{\alpha,\beta\gamma} &= \int_0^1 r_1^l e^{-\alpha r_1} dr_1 \int_0^\infty r_2^m e^{-\beta r_2} dr_2 \int_{|r_1 - r_2|}^{r_1 + r_2} \rho^n e^{-\gamma\rho} d\rho, \end{aligned} \tag{A13}$$

where $s = r_1 + r_2$. By means of recurrence relations these may be reduced to the I and S integrals defined above.