TENSOR FORCES AND THE THEORY OF HYDROGEN THREE

by

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Abstract

One of the most interesting problems in modern physics is the determination of the nature of "nuclear forces" or the interaction potentials between nucleons. The basic task of a phenomenological theory of nuclear forces is to find expressions for these potentials, with as few adjustable constants as possible, which will account for as many empirical facts as possible. In the present paper the fact of greatest interest is the binding energy of the triton, H^3.

Early attempts to account for the binding energy of the triton were fairly successful, but were based on the hypothesis of a central nuclear interaction potential which was unable to account for the presence of an electric deuteron quadrupole moment. The latter caused the introduction of tensor interaction potentials, which depend not only upon the relative locations of the nucleons but upon their relative orientations as well; it was then possible to set up a description of nuclear forces which accounted fairly well for the properties of the deuteron.

These forces proved to be ineffective in accounting for the triton binding energy, however. It was felt that further improvements could be introduced into the nuclear model by employing a Yukawa meson type of interaction and by using central and tensor forces of different ranges.

The dependence of the binding energy of the triton upon the range of the tensor interaction force is calculated using a nuclear interaction potential of the form:

$$V(r_{ij}) = -V_0\left\{\left[1 - \tfrac{1}{2}g + \tfrac{1}{2}g\,(\vec{\sigma}_i\cdot\vec{\sigma}_j)\right] J(r_{ij}) + \Gamma S_{ij}\,K(r_{ij})\right\}$$

$$\text{where}\quad S_{ij} = 3\,\frac{(\vec{\sigma}_i\cdot\vec{r}_{ij})(\vec{\sigma}_j\cdot\vec{r}_{ij})}{r_{ij}^2} - (\vec{\sigma}_i\cdot\vec{\sigma}_j)$$

$$J(r) = \frac{e^{-\beta r}}{\beta r}\ ,\qquad K(r) = \frac{e^{-\tau r}}{\tau r}$$

The value of β may be taken from proton-proton scattering data, and various values of τ assumed. The constants Γ and V_0 may be fixed, for a given β and τ, by data on binding energy and quadrupole moment of the deuteron. The constant g may be obtained from scattering data. For each value, a value of E is found.

To carry out the calculation, a Ritz variation method was employed, with a four term linear variation function representing one S state and three D states:

$$\Psi = A_S\,\Psi_S + A_D\,\Psi_D + A_{D'}\,\Psi_{D'} + A_{D''}\,\Psi_{D''}$$

$$\Psi_S = e^{-\frac{1}{2}\lambda(r_1+r_2+\rho)}\,\chi_s$$

$$\Psi_D = e^{-\frac{1}{2}\mu(r_1+r_2+\rho)}\left[r_1^2\,S_{13} + r_2^2\,S_{23}\right]\chi_s$$

$$\Psi_{D'} = (r_1-r_2)\,e^{-\frac{1}{2}\nu(r_1+r_2+\rho)}\left[r_1^2\,S_{13} - r_2^2\,S_{23}\right]\chi_s$$

$$\Psi_{D''} = (r_1-r_2)\,e^{-\frac{1}{2}\omega(r_1+r_2+\rho)}\left[3(\vec{\sigma}_1\cdot R)(\vec{\sigma}_3\cdot R) - R^2(\vec{\sigma}_1\cdot\vec{\sigma}_3)\right]\chi_s$$

where the spin wave function χ_s may be represented in conventional notation as

$$\chi_s = \frac{1}{\sqrt{2}} \left[\alpha(1)\ \beta(2) - \beta(1)\ \alpha(2) \right] \alpha(3)$$

and where r_1, r_2 and ρ are the respective internuclear distances between N and P, N and P, and N and N, and $\vec{R} \equiv \vec{r_1} \times \vec{r_2}$. In addition to E, values of the percentage D state P_D were calculated for comparison with magnetic moment data.

The parameters λ, μ, ν and ω were varied to obtain a minimum value of E for a given value of the tensor range parameter τ, and P_D calculated from the resulting wave function. Since the binding energy of the triton does not as yet have a universally accepted value, a table of τ (in units of $\frac{2.33}{2.76} \times 10^{13}$ cm^{-1})* and of P_D has been computed for a reasonable spread of values:

-E (Mev)	2.33 τ *	P_D
8.3	1.49	2.9
8.4	1.48	2.8
8.5	1.46	2.8

The value of E turns out to have a marked dependence upon the value of τ. However, it is necessary to realize that the value of τ affects the binding energy not only directly but also in large measure through restrictions imposed on Γ and V_0 through the requirements of compatibility with two-body data.

* $\beta = 1$ in these units.

It was found that all three of the D states made significant contributions to the energy; the smallest contribution, that of the D″ state, was of the order of 5 per cent.

The resulting percent D state P_D did not agree with the experimental value of 3.74 ± 0.06. However, the relation between P_D and the magnetic moments is not in a completely satisfactory state, since it was necessary to assume equality of total (not just nuclear) n-n and p-p forces. Also, the value of P_D may be low both because of the fact that an upper bound is all that was obtained for E with the variation method used and because there is a possibility that the value of β used was too small.

The value of τ determined corresponded to an equivalent triplet range for n-p scattering of 1.76 x 10^{-13} cm., in good agreement with experiment. This does not, however, furnish a very accurate check.

Further excellent experimental tests could be made by computing the H^3-He^3 Coulomb energy and the binding energy of the alpha particle.

Chapter I

INTRODUCTION

One of the most interesting problems in modern physics is the determination of the nature of "nuclear forces," or the terms in the quantum-mechanical Hamiltonian of a nuclear system which describe the interaction potentials between the nucleons. The basic task of a so-called phenomenological theory is to find expressions for these potentials, with as few adjustable constants as possible, which will account for as many empirical facts as possible.

The experimental data used to evaluate the adjustable constants and to check the resulting potentials are primarily of three types - cross-sections and angular distributions for various processes, nuclear moments, and nuclear binding energies. Due to the length of the calculations involved in the theory of even the lightest nuclei, one can only make use of data on nuclear systems containing a relatively small number of particles.

While all three types of data will be made use of in arriving at a set of interaction potentials, the primary interest of the present investigation is in the properties of the triton, H^3, and to some extent in its mirror nucleus He^3.

The triton does not exist in nature, but may be produced in a nuclear reaction such as

$$_7N^{15} + n \longrightarrow {_1H^3} + {_6C^{13}}.$$

It is β^- radioactive, transforming into He^3 with a half-life of about 12 years. The binding-energy difference between H^3 and He^3 has been accurately measured at 0.74 Mev by a determination of the maximum energy of the accompanying beta-ray spectrum; the calculation of this energy difference affords an excellent test of the wave function used in any phenomenological theory.

The most important property of H^3, from the standpoint of establishing a satisfactory theory, is its binding energy. The old value of 8.3 Mev was superseded by a value of 8.39 Mev(1), and there is reason to believe that a more correct value is 8.50 Mev as a result of a new determination of the value of the binding energy of the deuteron(2).

It is found that the ground state of H^3 has a spin of $\frac{1}{2}$. While this precludes the existance of a quadrupole moment, the magnetic moment of the triton furnishes another very useful check on the wave function used to describe the triton; the value of the magnetic moment

1 - Rosenfeld, Nuclear Forces, p. 501

2 - Bell and Elliott, Phys. Rev. 74, 1552 (1948)

of H^3 (and of He^3) set a requirement upon the composition of the ground-state wave function*.

Before the discovery of the electric deuteron quadrupole moment, scattering data and binding energy data could be accounted for reasonably well by the use of a central interaction potential. The most satisfactory research during this phase of nuclear theory was done by Rarita and Present in 1937(3). They set up a two-body interaction of the Majorana-Heisenberg type:

$$V(r_{ij}) = \left[(1-g)\ P_{ij} + g\ P_{ij}\ Q_{ij}\right] \quad J(r_{ij})$$

where P_{ij} was an operator exchanging the space coordinates of particles i and j, and Q_{ij} exchanged the spin coordinates; $J(r_{ij})$ was an exponential potential well. By inserting data from n-p scattering and from binding energy determinations of H^2 and H^3, they obtained a description of nuclear forces which would successfully account for p-p scattering data, the H^3-He^3 energy difference, and, within 20 per cent., the binding energy of He^4.

It was soon realized, however, that the central potentials would not be able to account for the electric quadrupole moment of the deuteron, discovered in 1939(4).

* For a detailed treatment see Chapter IV

3 - Rarita and Present, Phys. Rev. 51, 788 (1937)

4 - Kellogg, Rabi, Ramsey and Zacharias, Phys. Rev. 55, 318 (1939)

Further types of interaction were required. A search had previously been made[5] for types of particle interactions which would be invariant under rotation and reflection and did not explicitly involve the momenta of the interacting particles. It was found that there were six types of interaction which met the above conditions. Four of these were the simple exchange forces:

Ordinary (Wigner) forces, represented by 1,

Spin-exchange (Bartlett) forces, represented by $(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$,

Space-spin exchange (Heisenberg) forces, represented by $(\vec{\tau}_1 \cdot \vec{\tau}_2)$, and

Space-exchange (Majorana) forces, represemted by $(\vec{\tau}_1 \cdot \vec{\tau}_2)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$.

Two others, however, were of the " tensor " type, obtained by combining space and spin dyadics. They were of the form:

Tensor forces, represented by

$$S_{12} = \frac{3\,(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r})}{r^2} - (\vec{\sigma}_1 \cdot \vec{\sigma}_2)$$

Tensor exchange forces, represented by $(\vec{\tau}_1 \cdot \vec{\tau}_2)S_{12}$.

The above considerations led Rarita and Schwinger in 1941[6] to introduce a tensor force into the phenomenological two-body potential, giving it the form:

$$V(r) = \left[1 + \tfrac{1}{2}g - \tfrac{1}{2}g\,(\sigma_1 \cdot \sigma_2) + \gamma\, S_{12}\right] J(r)$$

5 - Wigner, Phys. Rev. 51, 106 (1937)

6 - Rarita and Schwinger, Phys. Rev. 59, 436, 556 (1941)

where J(r) was a square well potential. The presence of the tensor term in the potential implied that coupling would exist between the $^3S_1$ state and the higher states, so that the ground state would no longer be an S state. Considerations of parity and of the fact that S and J turned out to be good quantum numbers suggested to them that a suitable wave function would be the combination $^3S_1 + {}^3D_1$. Constants were fixed from data on slow n-p scattering, deuteron binding energy, and deuteron quadrupole moment. It was then possible to predict photoelectric disintegration cross section, radiative capture cross section for slow neutrons in hydrogen, and cross section for 2.8 Mev n-p scattering. The last was not in precise agreement with data available at that time, but is in excellent agreement with present data(7).

Since the Rarita-Schwinger theory had accounted so well for the properties of the deuteron, it was natural to apply the potential to a description of the properties of nuclear three- and four-body systems. Results proved to be in disagreement with experiment.

The first major research in applying the Rarita-Schwinger interaction potential to many-body systems was undertaken by Gerjuoy and Schwinger in 1942(8). In view of the importance of their work to the present investigation, it will be discussed in some detail.

7 - Bailey, Bennett, Bergstralh, Nuckolls, Richards and Williams, Phys. Rev. 70, 583 (1946)

8 - Gerjuoy and Schwinger, Phys. Rev. 61, 138 (1942)

The ground state of H^3 has angular momentum $J = \frac{1}{2}$. J is a constant of the motion since the interaction potential was chosen to be rotationally invariant, but S is no longer a constant of the motion. L is restricted by considerations of vector addition. Thus the ground state might include $^2S_{\frac{1}{2}}$, $^2P_{\frac{1}{2}}$, $^4P_{\frac{1}{2}}$ and $^4D_{\frac{1}{2}}$. Assuming arbitrarily $m = \frac{1}{2}$, the more important S state wave function would be

$$\chi_s = \frac{1}{\sqrt{2}} \left[\alpha(1)\,\beta(2) - \beta(1)\,\alpha(2) \right] \alpha(3)$$

(The other S state would have a space wave function vanishing at $r_1 = r_2$). To a first approximation, the tensor term in the potential would couple the important S state with D states; to a second approximation, with a rather complicated mixture of states. Since the percentage D state is quite small, one might expect a negligible amount of P state.

Suitable D states may be constructed by operating on χ_s with rotationally invariant operators obtained by combining the spin dyadic $\vec{\sigma}_1 \vec{\sigma}_3$ with certain space dyadics formed from $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_1 \times \vec{r}_2$. It turns out that four $^4D_{\frac{1}{2}}$ states may be formed in this manner, of which three prove to be independent. One spin wave function is odd in exchange of the neutrons, and the other two are even.

Gerjuoy and Schwinger chose as a trial variation function the sum of the S state and the odd D state, with Gaussian radial dependence, and performed a variation calculation using the potential of Rarita and Schwinger.

They obtained 32 % of the correct value of the binding energy of the triton, and 4 % D state. (Work on the alpha particle yielded 50% of the experimental value, and a check on the deuteron yielded 54%.)

Feshbach and Rarita(9) elaborated on the work of Gerjuoy and Schwinger by using a Hylleraas expansion. They obtained an estimated maximum of 40-50% of the experimental value of the binding energy of H^3.

Clapp(10) attacked the problem with several modifications. Firstly, he included a space-spin-exchange factor, which he considered to have only a slight effect upon the triton binding energy. Secondly, he included the other two previously neglected D states, which turned out to have a rather large effect, lowering the calculated binding energy by about 22%. He used a system of hyperspherical harmonics and a single radial variable, thus simplifying the problem of expansion in power series. His extrapolated value for the triton binding energy was about 70 % of the experimental value.

The preceding researches would imply that the square well was not too suitable as a description of the interaction potential. Furthermore, present-day scattering experiments require a different size of square well for singlet and triplet states, and different sizes for n-p and p-p interactions. Since any additional constants tend

9 - Feshbach and Rarita, Phys. Rev. 75, 1384 (1949)

10 - Clapp, Phys. Rev. 76, 873 (1949)

to defeat the purpose of a phenomenological theory, it would be well to consider other types of wells. Furthermore, as there is no a priori reason for assuming central and tensor force ranges the same, it would be advantageous to investigate the result of using potentials of different ranges in the hope that more than one correct result may be predicted by the addition of one more constant.

The most satisfactory well to use would appear to be the meson well. Some justification might arise from the fact that it is the only one derivable from any sort of basic theory. Considerably stronger justification arises, however, from the fact that its use, in connection with different ranges for central and tensor forces, allows prediction of a considerable number of experimental results and allows preservation of charge-independent nuclear forces. Preliminary calculations by Feshbach[11] show that this combination of wells will yield correct experimental results for n-p scattering at low and moderately high energies, neutron scattering by ortho- and para-hydrogen, deuteron binding energy, deuteron quadrupole moment, triton binding energy and photoelectric and photomagnetic disintegration of the deuteron. Furthermore, the meson well was shown to be capable of more satisfactory predictions regarding scattering experiments[12,13], and

11 - Feshbach, Phys. Rev. 76, 185(A) (1949)

12 - Bohm and Richman, Phys. Rev. 71, 567 (1947)

13 - Chew and Goldberger, Phys. Rev. 73, 1409 (1948)

recent results of Christian and Hart[14] on high-energy n-p scattering show a preference for a meson well as far as angular distribution is concerned, though their cross-section data tends to favor an exponential well.

In view of the above considerations, the present investigation will be based upon a meson well potential with different central and tensor ranges as used by Feshbach and Schwinger[15], of the form

$$V(r_{ij}) = - V_o \left[\left(1 - \tfrac{1}{2}g + \tfrac{1}{2}g\ (\vec{\sigma}_i \cdot \vec{\sigma}_j)\right) J(r_{ij}) + \Gamma S_{ij}\ K(r_{ij}) \right] \qquad (1)$$

$$J(r) = \frac{e^{-\beta r}}{\beta r} \qquad K(r) = \frac{e^{-\tau r}}{\tau r}$$

The value of β may be taken from p-p scattering data[16]. For a given β and τ , the constants V_o and Γ may be fixed by the binding energy and quadrupole moment of the deuteron.[15] The constant g, which occurs in the singlet well depth $V_o(1 - 2g)$, may be determined from scattering data(17).

The value of τ which yields the experimental value of the binding energy of H^3, and more generally the variation of the properties of the triton with the parameter τ, is the object of the present investigation. In particular, it is hoped that answers will be found for

14 - Christian and Hart, private communication

15 - Feshbach and Schwinger, to be published

16 - Hoisington, Share and Breit, Phys. Rev. 56, 884 (1939)

17 - Blatt and Jackson, Phys. Rev. 76, 18 (1949)

the following questions:

To what value of τ does the correct triton binding energy correspond?

How sensitive is the calculated binding energy to the value of τ ?

To what value of magnetic moment does the above determined value of τ correspond?

How sensitive is the calculated magnetic moment to the value of τ, or, more generally, how sensitive is the resulting wave function to the value of τ; both with regard to the values of the variational parameters and with regard to the percentages of various states present?

Chapter II

PROCEDURE

The major portion of the investigation consisted in setting up a Hamiltonian including the interaction potentials (1), choosing a suitable variation function, and applying the Ritz variation method to determine the upper bound to the lowest eigenvalue of the Hamiltonian.

A relative coordinate system shown in Fig. I at right was chosen, since the D state wave functions could then be constructed by operating on the S wave function with simple combinations of the tensor potential operators. The kinetic energy operator in this system turned out to be

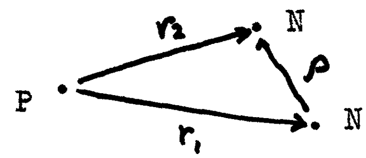

Fig. I - Coordinate system.

$$T = -\frac{\hbar^2}{M}\Bigg[\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial y_1^2}+\frac{\partial^2}{\partial z_1^2}\right)+\left(\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial y_2^2}+\frac{\partial^2}{\partial z_2^2}\right)$$
$$+\left(\frac{\partial^2}{\partial x_3^2}+\frac{\partial^2}{\partial y_3^2}+\frac{\partial^2}{\partial z_3^2}\right)+\left(\frac{\partial^2}{\partial x_2\partial x_3}+\frac{\partial^2}{\partial y_2\partial y_3}+\frac{\partial^2}{\partial z_2\partial z_3}\right)$$
$$-\left(\frac{\partial^2}{\partial x_3\partial x_1}+\frac{\partial^2}{\partial y_3\partial y_1}+\frac{\partial^2}{\partial z_3\partial z_1}\right)+\left(\frac{\partial^2}{\partial x_1\partial x_2}+\frac{\partial^2}{\partial y_1\partial y_2}+\frac{\partial^2}{\partial z_1\partial z_2}\right)\Bigg]+$$

where the subscript 3 has been used to designate the coordinates of ρ.

As discussed in Chapter I in regard to the work of Gerjuoy and Schwinger[8], the wave function was chosen to be a combination of S and D states; of the latter there are three independent ones, which we shall designate D, D' and D", which possess a total angular momentum of $\frac{1}{2}$. The specific wave functions used were as follows:

$$\Psi = A_S \psi_S + A_D \psi_D + A_{D'} \psi_{D'} + A_{D''} \psi_{D''}$$

$$\psi_S = f(r)\ \chi_s$$

$$\psi_D = g(r)\ \left[r_1^2\ S_{13} + r_2^2\ S_{23} \right] \chi_s$$

$$\psi_{D'} = h(r)\ \left[r_1^2\ S_{13} - r_2^2\ S_{23} \right] \chi_s$$

$$\psi_{D''} = p(r)\ \left[3\ (\vec{\sigma}_1 \cdot \vec{r}_1 X \vec{r}_2)(\vec{\sigma}_3 \cdot \vec{r}_1 X \vec{r}_2) - (\vec{r}_1 X \vec{r}_2)\cdot(\vec{r}_1 X \vec{r}_2)\ (\vec{\sigma}_1 \cdot \vec{\sigma}_3) \right] \chi_s$$

$$f(r) = e^{-\frac{1}{2}\lambda(r_1+r_2+\rho)}$$

$$g(r) = e^{-\frac{1}{2}\mu(r_1+r_2+\rho)}$$

$$h(r) = (r_1-r_2)\ e^{-\frac{1}{2}\nu(r_1+r_2+\rho)}$$

$$p(r) = (r_1-r_2)\ e^{-\frac{1}{2}\omega(r_1+r_2+\rho)}$$

The D states are chosen by the same criterion as those of Gerjuoy and Schwinger, but differ slightly in form since a different type of coordinate system is uded. The factors (r_1-r_2) were inserted into the last two radial wave functions to insure that the total wave function was antisymmetric in the coordinates of the two neutrons.

The theory of the Ritz variation method permits the automatic choice of optimum wave function coefficients through the solution of the secular determinant

$$\left| (_i \rangle H-E | _j) \right| = 0; \; i,j = S,D,D',D''. \qquad (2)$$

The optimum values of the coefficients λ , μ , ν , and ω are determined by finding the determinant which has as its solution the lowest value of E. Since this would be an extremely prolonged task without some means of estimating roughly the values of the parameters, some systematic method of attack must be formulated. In the present investigation, the actual computational procedure was as follows: Firstly, only the S term was considered, giving a 1 x 1 determinant which was easily soluble, and a value of λ found which gave a minimum value of E. Then the determinant was increased to a 2 x 2 determinant with the addition of terms involving the D state and, using the value of λ previously found, the value of μ was varied to yield a minimum energy. For the higher values of τ , the S state was found to be just barely bound, and the parameters λ and μ were varied simultaneously around the previously determined values. With reasonable values of λ and μ thus determined, the D' terms were added to form a 3 x 3 determinant and, keeping λ and μ constant, ν was varied for minimum E. Finally with λ , μ , and ν reasonably well determined, the entire 4 x 4 determinant was solved, and E minimized for variations in ω , with the other three variational parameters constant.

At that point one had a rough estimate of E, together with reasonably good values of λ, μ, ν and ω. The next step is to construct a net of points, varying those parameters upon which the energy seems to be especially dependent. In this case, the,S,D and D' states made quite large contributions to the energy, whereas the contribution made by the D" state was only of the order of 5 per cent. Furthermore, omission of either the D-D" or the D'-D" matrix elements had little effect on the energy. Consequently, it was decided to keep ω constant and make a net of 27 points with three values each of λ, μ, and ν. Finally, ω was varied slightly.

Determinants were set up for three values of τ, one of which was chosen to yield a value of E reasonably close to the experimental value. From the coefficients of the determinant corresponding to minimum E in each case we may deduce the relative amplitudes of the four wave functions and from that the percentage D state and magnetic moment.

For convenience in computation, the Hamiltonian was broken up into a sum of terms, each considered separately:

$$H = T + \text{(non-tensor potential terms)} + \text{(tensor potential terms)}$$

The general matrix element of the form $(i|H-E|j)$ was then written as the following sum:

$$(i|H-E|j) = 3.54688\,(i|KE|j) + (i|V|j)_{NT} + 2\,(i|T_{13}|j) + (i|T_{12}|j) - E\,(i|j)$$

The multiplying factor in front of the kinetic energy element $(i|KE|j)$ is a consequence of the units used (see Appendix D). The elements $(i|V|j)_{NT}$ represent the sum of three terms due to the three central-force interaction potentials, grouped together because of similarity. The three tensor elements, involving S_{13}, S_{23} and S_{12} respectively, were designated as $(i|T_{13}|j)$, $(i|T_{23}|j)$, and $(i|T_{12}|j)$ respectively, but advantage was taken of the fact that the first two were equal. The last element, a normalization element, existed in many of the off-diagonal terms of the determinant, since only the S state was orthogonal to all the others.

With respect to the actual algebraic manipulations involved in determining the forms of the (non-integrated) matrix elements, in general two methods were used, often one as a check on the other - a "brute force" method and a "symbolic" method.

The brute force method involved the expression of the matrix element as the scalar product of two terms, both terms expressed as sums of the eight orthogonal spin wave functions, with space-dependent coefficients. As an example, let us calculate $(D|D)$ (not integrated) by this method.

By making use of the Pauli spin operator equations, the D state spin-angular wave function,

$$\left[r_1^2\, S_{13} + r_2^2\, S_{23}\right] \frac{1}{\sqrt{2}}\left[\alpha(1)\,\beta(2)\,\alpha(3) - \beta(1)\,\alpha(2)\,\alpha(3)\right]$$

becomes the expression

$$\frac{1}{\sqrt{2}}\left\{\begin{array}{ll}
\alpha(1)\,\alpha(2)\,\alpha(3) & \left[3i(y_1z_1-y_2z_2)-3(x_1z_1-x_2z_2)\right] \\
\alpha(1)\,\alpha(2)\,\beta(3) & \left[2(z_1^2-z_2^2)-(x_1^2-x_2^2)-(y_1^2-y_2^2)\right] \\
\alpha(1)\,\beta(2)\,\alpha(3) & \left[2(z_1^2-z_2^2)-(x_1^2-x_2^2)-(y_1^2-y_2^2)\right] \\
\alpha(1)\,\beta(2)\,\beta(3) & \left[3i(y_1z_1-y_2z_2)+3(x_1z_1-x_2z_2)\right] \\
\beta(1)\,\alpha(2)\,\alpha(3) & \left[2(z_1^2-z_2^2)-(x_1^2-x_2^2)-(y_1^2-y_2^2)\right] \\
\beta(1)\,\alpha(2)\,\beta(3) & \left[3i(y_1z_1-y_2z_2)+3(x_1z_1-x_2z_2)\right] \\
\beta(1)\,\beta(2)\,\alpha(3) & \left[3i(y_1z_1-y_2z_2)+3(x_1z_1-x_2z_2)\right] \\
\beta(1)\,\beta(2)\,\beta(3) & \left[3(x_1^2-x_2^2)-3(y_1^2-y_2^2)+6i(x_1y_1-x_2y_2)\right]
\end{array}\right.$$

from whence $2(D|D) = 9(y_1z_1-y_2z_2)^2 + 9(x_1z_1-x_2z_2)^2 + \ldots$

$$= 12\,(r_1^4 + r_2^4 + r_1^2r_2^2 - 3(\vec{r}_1\cdot\vec{r}_2)^2)$$

or $(D|D) = 6\left[r_1^4 + r_2^4 + r_1^2r_2^2(1 - 3\cos^2\theta)\right]$

In the symbolic method, which is considerably more conventional, one expresses all operators in terms of the Pauli sigmas and uses standard identities to obtain an element in the form

$$(S \mid (\text{functions of coordinates alone}) + (\text{terms which, when operating on the S state spin wave function, make it orthogonal to itself}) \mid S)$$

$$= (\text{functions of coordinates alone}).$$

While the symbolic method is more elegant, it has the disadvantage that one algebraic error will lead to an incorrect result. In the "brute force" method, on the other hand, an error will often lead one to a final expression of the form $x_1^2 + y_1^2 - z_1^2$ + other terms which combine to form functions of r_1^2, r_2^2 and $r_1 \cdot r_2$ alone, from which one can at once tell that one has made am error in sign and approximately in what part of the computation one has made it.

Once the spin dependence has been eliminated from the matrix elements, integration over space coordinates may be carried out with reasonably standard techniques as discussed in Appendix A. Matrix elements, both before and after spatial integration, are listed in Appendices B and C, respectively.

Chapter III

RESULTS

The values of the four variation parameters*, triton binding energy*, and per cent. D state for the three values of τ used turned out to be:

τ	λ	μ	ν	ω	E	P_D
$\frac{1.30}{2.33}$	1.30	2.2	2.5	2.8	-1.118	2.5
$\frac{1.51}{2.33}$	1.25	2.2#	2.5#	2.8#	-0.986	2.9
$\frac{1.80}{2.33}$	1.16	2.2	2.5	2.8	-0.762	3.7

Corresponding values of τ and P_D for three values of triton binding energy which pretty well cover the experimental range are:

-E (Mev)	2.33 τ	P_D
8.3	1.49	2.9
8.4	1.48	2.8
8.5	1.46	2.8

The above values were computed from parabolas passing through the three experimental points which had the form*

$$E = -1.3704 - 0.1798\,(2.33\,\tau) + 0.2877\,(2.33\,\tau)^2$$

$$P_D = 3.376 - 2.894\,(2.33\,\tau) + 1.708\,(2.33\,\tau)^2.$$

* For units see Appendix D ; $\beta = 1$ in these units

\# Interpolated

The values of the constants Γ and V_o for each of the values of τ used are as follows:

τ	Γ	V_o
$\frac{1.30}{2.33}$	0.2259	6.6091
$\frac{1.51}{2.33}$	0.4074	6.0040
$\frac{1.80}{2.33}$	0.7894	4.9121

It was found that all three D states made significant contributions to the energy; the D" state, least important, contributed about 5%.

The corresponding equivalent triplet range for n-p scattering[15] is 1.76×10^{-13} cm, in good agreement with the most recent determination[18].

18 - Hughes, Ringo and Burgy, in press

Chapter IV

DISCUSSION

The most striking result obtained was the large sensitivity of the triton binding energy to variations in the range of the tensor force. In fact, the fractional variation of the binding energy is of the order of the fractional variation of the tensor range, allowing the value of β to be set rather definitely from experiment.

However, the fact that a variation in τ produces a large variation in E is not necessarily an indication that the tensor range per se has a large effect upon the properties of the system, for one must bear in mind that the values of Γ and V_0 were set by the value of τ from two-body data. Possibly the clearest example of this lies in the fact that, while the S-state energy does not explicitly depend upon τ , the variation of τ between the two extreme cases studied produced a sufficient change in the value of V_0 to vary the S state energy from about -0.6 to about zero. The total energy, in contrast, varied only by about 0.36.

The preceding argument may be brought out less strikingly but possibly more satisfactorily by a set of calculations involving the S and D (but not D' or D") wave functions, for which the values of Γ and V_0 were held constant while the parameter τ was varied explicitly. For the variation in τ mentioned (from 1.3/2.33 to 1.8/2.33), the energy changed only by 0.15; use of the correct values of Γ and V_0 quadrupled the energy change. One must also consider that an increase in τ does not only decrease the range of a potential well but also its depth, so that τ is not purely of the nature of a "range" parameter.

It is of further interest to note that the optimum value of λ, the S state variation parameter, which is affected by τ only indirectly through V_0 and through a small amount of coupling, varies as τ is varied, whereas the D state parameters μ, ν and ω are unaffected. In general, then, one may conclude that the value of τ affects the binding energy not only directly but in large measure through restrictions imposed upon other parameters through the requirements of compatibility with other data.

The binding energy, however, did not furnish any experimental test of the theory (other than that it was possible to find a reasonable value of tensor range which would give the experimental energy); binding energy data was used simply to set the value of τ. One experimental test, which may be made with ease but interpreted with reservations, is the checking of the theoretical P_D value with experimental data on magnetic moments. While P_D is as sensitive as E to variations in τ, it is less useful for comparison with data due to the somewhat uncertain relation between P_D and the magnetic moment.

If the like particles are designated by (1) and (2) in each case, the magnetic moments of H^3 and He^3 may be expressed respectively as[19]

$$\mu_H = \left\langle L_{3z} + 2\mu_n (S_{1z} + S_{2z}) + 2\mu_p (S_{3z}) \right\rangle$$

$$\mu_{He} = \left\langle L_{1z} + L_{2z} + 2\mu_p (S_{1z} + S_{2z}) + 2\mu_n (S_{3z}) \right\rangle$$

It is apparent by inspection that, whereas the evaluation of either moment separately requires detailed knowledge of the properties of the particular wave functions, great simplification results if one is interested in computing only the sum of the moments, assuming that the n-n and p-p interactions are identical

$$\mu \equiv \mu_H + \mu_{He} = \left\langle L_z + 2(\mu_n + \mu_p) S_z \right\rangle$$

Treating L and S as vectors and setting them proportional to J allows the above to be put in terms of constants of the motion

$$\mu = m \left[2(\mu_n + \mu_p) - 2(\mu_n + \mu_p - \tfrac{1}{2}) \times \frac{J(J+1)+L(L+1)-S(S+1)}{2J(J+1)} \right]$$

This expression may be evaluated for the four states which might be present and expressed as

$$\mu = \mu_n + \mu_p - 200 (\mu_n + \mu_p - \tfrac{1}{2}) \frac{3 P_D - P_{4P} + 2 P_{2P}}{3}$$

where the last three terms refer respectively to percentages of $^4D_{\frac{1}{2}}$, $^4P_{\frac{1}{2}}$ and $^2P_{\frac{1}{2}}$ states present in the ground state.

19 - Sachs and Schwinger, Phys. Rev. 70, 41 (1946)

If, in addition to the assumption of equality of n-n and p-p interactions, we assume that the ground states of H^3 and He^3 are composed of S and D (but not P) components, we may arrive at an expression for PD in terms of experimental data:

$$P_D = \frac{(\mu_n + \mu_p) - (\mu_H + \mu_{He})}{2\,(\mu_n + \mu_p - \frac{1}{2})} \times 100 \text{ per cent.}$$

These four moments have been measured precisely and are:

Moment	Value in n.m.	Reference
μ_n	- 1.91354 ± 0.00013	20
μ_p	2.79353 ± 0.00014	21
μ_{H^3}	2.97968 + 0.00015	22
μ_{He^3}	(-)2.12815	23

Errors for the first three quantities were computed from the convenient table in reference 21. The error in 23 appeared to be smaller than the others by an order of magnitude.

The resulting PD turned out to be 3.74 ± 0.06, definitely above the predicted value of 2.8 obtained in the present thesis. It must be remembered that two assumptions were made, however, one that the n-n and p-p interactions

20 - Bloch, Nicodemus and Staub, Phys. Rev. 74, 1025 (1948)

21 - Taub and Kusch, Phys. Rev. 75, 1481 (1948)

22 - Bloch, Graves, Packard and Spence, Phys. Rev. 71, 551 (1947)

23 - Anderson, Phys. Rev. 76, 1460 (1949)

were identical, and another that only S and D states were present.

With regard to the first, the assumption of charge independence of nuclear forces does not mean equality of the total n-n and p-p forces but only of the specifically nuclear portion. The effect of the Coulomb force is to weaken the p-p interaction; Coulomb repulsion would mean that the protons would tend on the average to be farther apart, favoring a larger proportion of D state. Since the Coulomb perturbation energy is about 9% of the system energy, and since the increase in P_D is proportional not to the square of the additional D amplitude but to the product of original and additional amplitude, and since the perturbation would favor the D state, one might expect an increase of P_D of an appreciable fraction of one per cent. With regard to the second, P states will appear, for the treatment of the tensor force as a perturbation will predict their entrance in second order, and even a small fraction of a per cent. of ^2P state would be of help in closing the small gap between theory and experiment.

Whereas the experimental value of the sum of the magnetic moments of H^3 and He^3 was of some aid as a check on the calculations, experimental data on individual moments, in the present state of the theory, would appear to be of no help at all. The work of Sachs and Schwinger(19), based on reasonable wave functions, yielded a triton moment smaller than the proton moment, whereas it was seen that the triton moment is actually larger than the proton moment. Of the two proposals put forth to account for this - a contribution due to exchange currents produced by a pseudoscalar meson field(24) and the presence of an extremely large admixture of P and D components in the ground state wave function(25) - the former is more in agreement with experiment. Unfortunately, the evaluation of Villars is very rough, and the result could not be used for a quantitative check on P_D.

It is of interest to note that the values of P_D for the triton are quite close to those obtained for the deuteron by Feshbach and Schwinger(15).

The value of the effective triplet scattering length, while furnishing a good check, is not a very precise method of verifying the value of τ. A change in the latter from 1.3/2.33 to 1.8/2.33 produces a change(15) in the former of only about 5 %, whereas the per cent. error of a suitable scattering experiment might be about half that value.

With respect to all of the above data, it must be remembered that the present calculation yielded an upper bound to the energy, and that it can hardly be said that convergence was extremely rapid. Furthermore, it might be noted that any decrease in this bound would result in better agreement with experiment as far as P_D is concerned. To set a lower bound by computation of $\langle H^2 \rangle$ using the actual wave function would involve tremendous computational difficulties, while use of a simpler wave function such as

24 - Villars, Phys. Rev. 72, 256 (1947)

25 - Sachs, Phys. Rev. 72, 312 (1947)

ψ_s might not yield a very useful result. The introduction of one or more extra parameters by splitting up the present wave functions into members having different exponential space dependence would not require too much algebraic manipulation, and might be especially applicable to the S state, since the extra work involved would be simple, fewer extra elements would be added in comparison with splitting up of one of the D states, and the parameter λ is by far the most critical of the factors as far as the variational determination of energy is concerned. Addition of the second S state or even of a P state might be another possibility.

One must also consider that the value of β was taken from old p-p scattering data, and there is reason to believe that it should be somewhat larger.[26] This would mean a smaller value of Γ and a larger value of V_0 for the same value of τ, and thus a more negative value of E. Again this would bring the result for P_D closer to experiment.

A straightforward and very effective check on the present work would be the application of the resulting wave function to the calculation of the H^3-He^3 Coulomb energy. Another excellent check would be the application of the interaction potentials to the alpha particle; due to the accuracy to which the binding energy of He^4 is known, a definitive test of the present theory would be obtained which would be well worth the large amount of algebra involved.

26 - Bethe, Phys. Rev. 76, 38 (1949)

Further work should surely be done on the effect of converting from a neutral to a symmetric meson theory, i.e., premultiplying the interaction potential by a factor $-\frac{1}{3}(\vec{\tau}_i \cdot \vec{\tau}_j)$ as was done by Clapp[10].

There remain considerations involving the finite velocity of the nucleons. The velocity distribution might well be investigated by a transformation of the wave functions to momentum space. Breit[27] has derived corrections to the interaction Hamiltonian on the basis of equations invariant to order v^2/c^2, including corrections for a Thomas spin-orbit coupling, a Larmor spin-orbit coupling, and an interaction analogous to that between two magnetic dipoles. Primakoff and Holstein showed that there also exist many-body potentials; three-body interactions are of the order of v/c times the two-body potentials[28]. It is expected that these corrrections would be of especial importance for the D states.

27 - Breit, Phys. Rev. 51, 248, 778 (1937)
Phys. Rev. 53, 153 (1938)

28 - Primakoff and Holstein, Phys. Rev. 55, 1218 (1939).

Appendix A

Methods of Integration

Since all of the quantities to be integrated may be expressed as $f(r_1,r_2,\theta)$ or as $f(r_1,r_2,\rho)$, the simplest-appearing scheme of integration would appear to be the use of one of these sets of variables as the integration variables. This is indeed possible, and the resulting integral would be of the form

$$\int f(r_1,r_2,\theta)\, d\tau = 4\int_0^\infty r_1^2\, dr_1 \int_0^\infty r_2^2\, dr_2 \int_0^\pi \sin\theta\, d\theta \times f\,(r_1,r_2,\theta)$$

or its equivalent

$$\int f(r_1,r_2,\rho)\, d\tau = 4\int_0^\infty r_1\, dr_1 \int_0^\infty r_2\, dr_2 \int_{|r_1-r_2|}^{r_1+r_2} \rho\, d\rho \times f\,(r_1,r_2,\rho)$$

Inspection of the matrix elements, however, reveal a combination of f, g, h or p, all of which contain the factor ρ in an exponential. Integration of such quantities by the second method above, let alone by the first, would be extremely unwieldy.

Many of the integrals contain exponentials of the form $e^{-a(r_1+r_2)-b\rho}$. This symmetry in allows the use of the Hylleraas system explained in detail in Rarita and Present(3). In this system, one chooses as an integration scheme the quantities:

$$s = (r_1 + r_2), \quad t = r_1 - r_2, \quad \rho \text{ as before.}$$

One then integrates in the order

$$\int f(s,t,\rho)\, d\tau = \int_0^\infty ds \int_0^s d\rho \int_0^\rho dt\, \rho(s^2-t^2)\, f(s,t,\rho)$$

The results may be expressed in terms of functions

$$H^{a,b}_{j,k} = \int_0^\infty s^j\, e^{-as}\, ds \int_0^s \rho^k\, e^{-b\rho}\, d\rho$$

which may be easily evaluated by the reduction equation

$$H^{a,b}_{j,k} = \frac{1}{a}\left[S^{a+b}_{j+k} + j\; H^{a,b}_{j-1,k} \right]$$

$$S^c_m = \frac{c!}{m^{c+1}}$$

As an example, let us use this method to compute the normalization element $(S|S)$.

$$(S|S) = \int_0^\infty e^{-\lambda s}\, ds \int_0^s e^{-\lambda\rho}\, d\rho \int_0^\rho dt\, \rho\,(s^2-t^2)$$

$$= \int_0^\infty e^{-\lambda s}\, ds \int_0^s e^{-\lambda\rho}\, d\rho\, \left(s^2\rho^2 - \tfrac{1}{3}\rho^4\right)$$

$$= H^{\lambda\lambda}_{2,2} - \frac{1}{3} H^{\lambda\lambda}_{0,4}$$

But $H^{\lambda\lambda}_{0,4} = \dfrac{1}{\lambda} S^{2\lambda}_{4} = \dfrac{4!}{\lambda(2\lambda)^5} = \dfrac{3}{4\lambda^6}$

and $H_{2,2} = \dfrac{1}{\lambda} S^{2\lambda}_{4} + \dfrac{2}{\lambda^2} S^{2\lambda}_{3} + \dfrac{2}{\lambda^3} S^{2\lambda}_{2}$

$$= \frac{4!}{\lambda(2\lambda)^5} + \frac{2\cdot 3!}{\lambda^2(2\lambda)^4} + \frac{2\cdot 2!}{\lambda^3(2\lambda)^3} = \frac{3+3+2}{4\lambda^6}$$

or $(S\ S) = \dfrac{8-1}{4\lambda^6} = \dfrac{7}{4\lambda^6}$

For integrals where the exponentials in r_1 and r_2 have different coefficients (or where it is desired to check a Rarita-Present type of integration) it is generally simpler to use the method of Coolidge and James[29]. This system makes use of the integration variables

$$\xi = r_1 + r_2 - \rho \ , \ \eta = r_1 - r_2 + \rho \ , \ \zeta = -r_1 + r_2 + \rho$$

and an integration scheme in which all variables are integrated from zero to infinity:

$$\int f(\xi,\eta,\zeta)\, d\tau = \frac{1}{8}\int_0^\infty d\xi \int_0^\infty d\eta \int_0^\infty d\zeta \; f(\xi,\eta,\zeta) \times (\xi+\eta)(\xi+\zeta)(\eta+\zeta)$$

As an example, let compute the normalization element $(S|S)$ by this method also.

$$\begin{aligned}(S|S) &= \frac{1}{8}\int_0^\infty e^{-\lambda\xi} d\xi \int_0^\infty e^{-\lambda\eta} d\eta \int_0^\infty e^{-\lambda\zeta} d\zeta\, (\xi+\eta)(\xi+\zeta)(\eta+\zeta) \\ &= \frac{1}{8}\int_0^\infty e^{-\lambda\xi} d\xi \int_0^\infty e^{-\lambda\eta} d\eta \int_0^\infty e^{-\lambda\zeta} d\zeta \ \times \\ &\quad (\xi^2\eta + \xi\eta^2 + \xi^2\zeta + \xi\zeta^2 + \eta^2\zeta + \eta\zeta^2 \\ &\quad + 2\xi\eta\zeta) \\ &= \frac{1}{8}\,\frac{1}{\lambda^6}\left[(2!1!0!)(6) + (1!1!1!)(2)\right] \\ &= \frac{1}{8}\,\frac{1}{\lambda^6}\,(12+2)\end{aligned}$$

or $(S\ S) = \dfrac{7}{4\lambda^6}$ as before.

29 - Coolidge and James, Phys. Rev. 51, 885 (1937)

During the course of the latter integrations, situations arose in which one was faced with an integral of the type

$$\int_0^\infty e^{-a\xi}\, d\xi \int_0^\infty e^{-a\eta}\, d\eta \quad \frac{f(\xi,\eta)}{(\xi+\eta)^2}$$

where the integration over ζ had been successfully carried out and where $f(\xi, \eta)$ was not divisible by $(\xi+\eta)$. In order to avoid any approximations by the use of infinite series and possible convergence difficulties, it was decided to carry out simultaneous integration over ξ and η using a set of integration variables

$$y = \xi + \eta \quad , \; x = \xi - \eta$$

which transformed the preceding integral to

$$\frac{1}{2} \int_0^\infty e^{-ay} \; \frac{dy}{y^2} \int_{-y}^{y} f(x,y)\, dx .$$

The nature of the f(x,y) was such that the above method was always sufficient to carry out the integrations exactly.

Appendix B

Matrix Elements, Not Integrated

Normalization elements:

$$(S|S) = \int f^2 \, d\tau$$

$$(S|D) = 0$$

$$(S|D') = 0$$

$$(S|D'') = 0$$

$$(D|D) = \int g^2 \, d\tau \; 6 \left[r_1{}^4 + r_2{}^4 + r_1{}^2 r_2{}^2 (1 - 3 \cos^2\theta) \right]$$

$$(D|D') = \int g \, h \, d\tau \; 6 \left[r_1{}^4 - r_2{}^4 \right]$$

$$(D|D'') = \int g \, p \, d\tau \, (-3)(r_1{}^2 - r_2{}^2) r_1{}^2 r_2{}^2 \, (1 - \cos^2\theta)$$

$$(D'|D') = \int h^2 \, d\tau \; 6 \left[r_1{}^4 + r_2{}^4 - r_1{}^2 r_2{}^2 (1 - 3 \cos^2\theta) \right]$$

$$(D'|D'') = \int h \, p \, d\tau \, (-3)(r_1{}^2 + r_2{}^2) r_1{}^2 r_2{}^2 \, (1 - \cos^2\theta)$$

$$(D''|D'') = \int p^2 \, d\tau \; 6 \left[r_1{}^2 r_2{}^2 \, (1 - \cos^2\theta) \right]^2$$

Kinetic energy elements:

Let
$$P(u,v) \equiv \frac{u}{r_1^2}\frac{\partial}{\partial r_1}\left(r_1^2\frac{\partial v}{\partial r_1}\right) + \frac{u}{r_2^2}\frac{\partial}{\partial r_2}\left(r_2^2\frac{\partial v}{\partial r_2}\right) + \frac{u}{\rho^2}\frac{\partial}{\partial \rho}\left(\rho^2\frac{\partial v}{\partial \rho}\right) + \frac{\vec{r}_1\cdot\vec{r}_2}{r_1\, r_2}\, u\,\frac{\partial^2 v}{\partial r_1 \partial r_2} - \frac{\vec{r}_1\cdot\vec{\rho}}{r_1\,\rho}\, u\,\frac{\partial^2 v}{\partial r_1 \partial \rho} + \frac{\vec{r}_2\cdot\vec{\rho}}{r_2\,\rho}\, u\,\frac{\partial^2 v}{\partial r_2 \partial \rho}$$

Then:

$$(S|KE|S) = -\int d\tau\; P(f,f)$$

$$(S|KE|D) = 0$$

$$(S|KE|D') = 0$$

$$(S|KE|D'') = 0$$

$$(D|KE|D) = -\int d\tau \Big\{ \Big[P(g,g) + \frac{2\,g}{\rho}\frac{\partial g}{\partial \rho} \Big] \times 6\left[r_1^4 + r_2^4 + r_1^2 r_2^2 (1 - 3\cos^2\theta)\right] + \frac{4g}{r_1}\frac{\partial g}{\partial r_1}\left[6r_1^4 + 3r_1^2 r_2^2(1 - 3\cos^2\theta)\right] + \frac{4g}{r_2}\frac{\partial g}{\partial r_2}\left[6r_2^4 + 3r_1^2 r_2^2(1 - 3\cos^2\theta)\right] \Big\}$$

$$(D|KE|D') = -\int d\tau \Big\{ \Big[P(g,h) \times 6\,(r_1^4 - r_2^4) \Big] + \frac{4g}{r_1}\frac{\partial h}{\partial r_1}\left[6r_1^4 + 3r_1^2 r_2^2(1 - 3\cos^2\theta) + 3\,(r_1^2 - r_2^2)\, r_1 r_2 \cos\theta\right] + \frac{4g}{r_2}\frac{\partial h}{\partial r_2}\left[-6r_2^4 - 3r_1^2 r_2^2(1 - 3\cos^2\theta) + 3\,(r_1^2 - r_2^2)\, r_1 r_2 \cos\theta\right] + \frac{4g}{\rho}\frac{\partial h}{\partial \rho}\left[3\,(r_1^4 - r_2^4) - 6(r_1^2 - r_2^2)\, r_1 r_2 \cos\theta\right] \Big\}$$

$$(D|KE|D'') = -\int d\tau \Bigg\{ \left[P(g,p) + \frac{4g}{r_1}\frac{\partial p}{\partial r_1} + \frac{4g}{r_2}\frac{\partial p}{\partial r_2} + \frac{4g}{\rho}\frac{\partial p}{\partial \rho} \right] \times \left[(-3)(r_1^2 - r_2^2)\, r_1^2 r_2^2\, (1 - \cos^2\theta) \right] + gp \left[\begin{array}{l} -12\,(r_1^4 - r_2^4) \\ +12\,(r_1^2 - r_2^2)\, r_1 r_2 \cos\theta \end{array} \right] \Bigg\}$$

$$(D'|KE|D') = -\int d\tau \Bigg\{ \left[P(h,h) \right] \times 6 \left[r_1^4 + r_2^4 - r_1^2 r_2^2\, (1 - 3\cos^2\theta) \right] + \frac{4h}{r_1}\frac{\partial h}{\partial r_1} \left[\begin{array}{l} 6r_1^4 - 3r_1^2 r_2^2 (1 - 3\cos^2\theta) \\ + 3(r_1^2 + r_2^2)\, r_1 r_2 \cos\theta \end{array} \right] + \frac{4h}{r_2}\frac{\partial h}{\partial r_2} \left[\begin{array}{l} 6r_2^4 - 3r_1^2 r_2^2 (1 - 3\cos^2\theta) \\ +3\,(r_1^2 + r_2^2)\, r_1 r_2 \cos\theta \end{array} \right] + \frac{4h}{\rho}\frac{\partial h}{\partial \rho} \left[\begin{array}{l} 3\,(r_1^4 + r_2^4) \\ -3\, r_1^2 r_2^2\, (1 - 3\cos^2\theta) \\ -\,6\,(r_1^2 + r_2^2)\, r_1 r_2 \cos\theta \end{array} \right] \Bigg\}$$

$$(D'|KE|D'') = -\int d\tau \Bigg\{ \left[P(h,p) + \frac{4h}{r_1}\frac{\partial h}{\partial r_1} + \frac{4h}{r_2}\frac{\partial h}{\partial r_2} + \frac{4h}{\rho}\frac{\partial h}{\partial \rho} \right] \times \left[(-3)(r_1^2 + r_2^2)\, r_1^2 r_2^2\, (1 - \cos^2\theta) \right] + hp \left[\begin{array}{l} -12\,(r_1^4 + r_2^4) \\ -12\, r_1^2 r_2^2\, (1 - 3\cos^2\theta) \\ +12\,(r_1^2 + r_2^2)\, r_1 r_2 \cos\theta \end{array} \right] \Bigg\}$$

$$(D''|KE|D'') = -\int d\tau \Bigg\{ \left[P(p,p) + \frac{4p}{r_1}\frac{\partial p}{\partial r_1} + \frac{4p}{r_2}\frac{\partial p}{\partial r_2} + \frac{4p}{\rho}\frac{\partial p}{\partial \rho} \right] \times 6 \left[r_1^2 r_2^2\, (1 - \cos^2\theta) \right]^2 + p^2 \left[\begin{array}{l} 6(r_1^2 + r_2^2) r_1^2 r_2^2\, (1 - \cos^2\theta) \\ -6\, r_1 r_2 \cos\theta\, (r_1^2 r_2^2)(1 - \cos^2\theta) \end{array} \right] \Bigg\}$$

Non-tensor potential elements:

$$(S|V|S)_{NT} = L^S(13) + L^S(23) + L^S(12)$$

$$L^S(13) = -V_o\ (1 - \tfrac{1}{2}g) \int f^2\ J(r_1)\ d\tau$$

$$L^S(23) = -V_o\ (1 - \tfrac{1}{2}g) \int f^2\ J(r_2)\ d\tau\ ,$$

$$L^S(12) = -V_o\ (1 - 2g) \int f^2\ J(\rho)\ d\tau$$

With the exception of the S-S elements listed above, the non-tensor potential elements are the same as the corresponding normalization elements, premultiplied by $-V_o$, and with a factor of $\left[J(r_1) + J(r_2) + J(\rho)\right]$ inserted in the integrand. As a typical example,

$$(D|V|D')_{NT} = L^{DD'}(13) + L^{DD'}(23) + L^{DD'}(12)$$

$$L^{DD'}(13) = -V_o \int g\ h\ J(r_1)\ (6\ r_1^4 - 6\ r_2^4)\ d\tau$$

$$L^{DD'}(23) = -V_o \int g\ h\ J(r_2)\ (6\ r_1^4 - 6\ r_2^4)\ d\tau$$

$$L^{DD'}(12) = -V_o \int g\ h\ J(\rho)\ (6\ r_1^4 - 6\ r_2^4)\ d\tau$$

T_{13} potential elements:

$$(S|T_{13}|S) = 0$$

$$(S|T_{13}|D) = -\Gamma V_o \int f\ g\ K(r_1) \left[6r_1^2 + (3-9\cos^2\theta)r_2^2\right] d\tau$$

$$(S|T_{13}|D') = -\Gamma V_o \int f\ h\ K(r_1) \left[6r_1^2 - (3-9\cos^2\theta)r_2^2\right] d\tau$$

$$(S|T_{13}|D'') = +\Gamma V_o \int f\ p\ K(r_1) \left[3r_1^2 r_2^2 (1-\cos^2\theta)\right] d\tau$$

$$(D|T_{13}|D) = -\Gamma V_o \int g^2\ K(r_1) \left[-12\ r_1^4 + 6(r_2^4 - r_1^2 r_2^2)(1-3\cos^2\theta)\right] d\tau$$

$$(D|T_{13}|D') = -\Gamma V_o \int g\ h\ K(r_1) \left[-12r_1^4 - 6r_2^4(1-3\cos^2\theta)\right] d\tau$$

$$(D|T_{13}|D'') = -\Gamma V_o \int g\ p\ K(r_1) \left[6r_1^4 r_2^2 (1-\cos^2\theta) + 3r_1^2 r_2^4 (4 - 10\cos^2\theta + 6\cos^4\theta)\right] d\tau$$

$$(D'|T_{13}|D') = -\Gamma V_o \int h^2\ K(r_1) \left[-12\ r_1^4 + 12\ r_1^2 r_2^2 (1 - 3\cos^2\theta) + 6\ r_2^4 (1 - 3\cos^2\theta)\right] d\tau$$

$$(D'|T_{13}|D'') = -\Gamma V_o \int h\ p\ K(r_1) \left[6r_1^4 r_2^2 (1-\cos^2\theta) - 3r_1^2 r_2^4 (4 - 10\cos^2\theta + 6\cos^4\theta)\right] d\tau$$

$$(D''|T_{13}|D'') = -\Gamma V_o \int p^2\ K(r_1)\ 6\left[r_1^2 r_2^2 (1-\cos^2\theta)\right]^2 d\tau$$

T_{12} potential elements:

$$(S|T_{12}|S) = 0$$

$$(S|T_{12}|D) = 0$$

$$(S|T_{12}|D') = 0$$

$$(S|T_{12}|D'') = 0$$

$$(D|T_{12}|D) = -\Gamma V_0 \int g^2 K(\rho) \times \Big\{ 12 \left[r_1^4 + r_2^4 + r_1^2 r_2^2 \left(\frac{3\cos^2\theta - 1}{2} \right) \right] - \frac{12}{\rho^2} \begin{bmatrix} 2r_1^6 + 2r_2^6 + r_1^2 r_2^2 (r_1^2 + r_2^2) \\ + 2\, r_1^2 r_2^2 (r_1 r_2 \cos\theta) \\ - 4\,(r_1^4 + r_2^4)(r_1 r_2 \cos\theta) \end{bmatrix} \Big\} d\tau$$

$$(D|T_{12}|D') = -\Gamma V_0 \int g\, h\, K(\rho) \times \Big\{ 12\,(r_1^4 - r_2^4) - \frac{12}{\rho^2} \begin{bmatrix} 2r_1^6 - 2r_2^6 + \tfrac{1}{2} r_1^2 r_2^2 (r_1^2 - r_2^2) \\ -4\,(r_1^4 - r_2^4)(r_1 r_2 \cos\theta) \\ +\tfrac{3}{2}\,(r_1^2 - r_2^2)(r_1^2 r_2^2 \cos^2\theta) \end{bmatrix} \Big\} d\tau$$

$$(D|T_{12}|D'') = -\Gamma V_0 \int g\, p\, K(\rho)\; 6\,(r_1^2 r_2^2)(r_1^2 - r_2^2) \times (1 - \cos^2\theta)\; d\tau$$

$$(D'|T_{12}|D') = -\Gamma V_o \int h^2 K(\rho) \Bigg\{ 12 \left[r_1^4 + r_2^4 + r_1^2 r_2^2 \left(\frac{1 - 3\cos^2\theta}{2} \right) \right] - \frac{12}{\rho^2} \Big[2r_1^6 + 2r_2^6 - 4(r_1^4 + r_2^4)(r_1 r_2 \cos\theta) - 2 r_1^2 r_2^2 (r_1 r_2 \cos\theta) + 3(r_1^2 + r_2^2) r_1^2 r_2^2 \cos^2\theta \Big] \Bigg\} d\tau$$

$$(D'|T_{12}|D'') = -\Gamma V_o \int h\, p\, K(\rho) \times \left\{ \left[6 (r_1^2 + r_2^2) r_1^2 r_2^2 (1 - \cos^2\theta) \right] - \frac{36}{\rho^2} \left[r_1^2 r_2^2 (1 - \cos^2\theta) \right]^2 \right\} d\tau$$

$$(D''\ T_{12}\ D'') = -\Gamma V_o \int p^2 K(\rho)\ 6 \left[r_1^2 r_2^2 (1 - \cos^2\theta) \right]^2 d\tau$$

Appendix C

Matrix Elements, Integrated

Normalization elements:

$$(S|S) = \frac{7}{4\lambda^6}$$

$$(S|D) = 0$$

$$(S|D') = 0$$

$$(S|D'') = 0$$

$$(D|D) = 1232 \frac{6!}{(2\mu)^{10}}$$

$$(D|D') = 4576 \frac{6!}{(\mu+\nu)^{11}}$$

$$(D|D'') = -14976 \frac{6!}{(\mu+\omega)^{13}}$$

$$(D'|D') = \frac{164736}{5} \frac{6!}{(2\nu)^{12}}$$

$$(D'|D'') = -\frac{708864}{5} \frac{6!}{(\nu+\omega)^{14}}$$

$$(D''|D'') = 82944 \frac{6!}{(2\omega)^{16}}$$

Kinetic energy elements:

$$(S|KE|S) = \frac{15}{8\chi^4}$$

$$(S|KE|D) = 0$$

$$(S|KE|D') = 0$$

$$(S|KE|D'') = 0$$

$$(D|KE|D) = 318\,\frac{6!}{(2\mu)^8}$$

$$(D|KE|D') = \frac{6!}{(\mu+\nu)^{11}}\left[4560\,\mu\nu - 240\,\mu^2\right]$$

$$(D|KE|D'') = \frac{6!}{(\mu+\omega)^{13}}\left[\frac{26048}{5}\,\mu^2 - \frac{54208}{5}\,\mu\omega\right]$$

$$(D'|KE|D') = \frac{47584}{5}\,\frac{6!}{(2\nu)^{10}}$$

$$(D'|KE|D'') = \frac{6!}{(\nu+\omega)^{14}}\left[\frac{163968}{5}\nu^2 - \frac{607488}{5}\nu\omega - \frac{12672}{5}\omega^2\right]$$

$$(D''|KE|D'') = \frac{7068672}{5}\,\frac{6!}{(2\omega)^{14}}$$

Non-tensor potential elements:

$$(S|V|S)_{NT} = -\frac{3\,V_o(1-g)}{4}\left[\frac{8}{\lambda^3(2\lambda+1)^2}+\frac{16}{\lambda^2(2\lambda+1)^3}+\frac{16}{\lambda(2\lambda+1)^4}\right]$$

$$(D|V|D)_{NT} = -\,6!\,V_o\left[\frac{3/4}{\mu^7(2\mu+1)^2}+\frac{3/2}{\mu^6(2\mu+1)^3}+\frac{7/2}{\mu^5(2\mu+1)^4}+\frac{8}{\mu^4(2\mu+1)^5}+\frac{16}{\mu^3(2\mu+1)^6}+\frac{28}{\mu^2(2\mu+1)^7}+\frac{36}{\mu(2\mu+1)^8}\right]$$

$$(D|V|D')_{NT} = -\,6!\,V_o\left[\frac{672}{(\mu+\nu)^8(\mu+\nu+1)^2}+\frac{480}{(\mu+\nu)^7(\mu+\nu+1)^3}+\frac{352}{(\mu+\nu)^6(\mu+\nu+1)^4}+\frac{288}{(\mu+\nu)^5(\mu+\nu+1)^5}+\frac{128}{(\mu+\nu)^4(\mu+\nu+1)^6}+\frac{64}{(\mu+\nu)^3(\mu+\nu+1)^7}+\frac{320}{(\mu+\nu)^2(\mu+\nu+1)^8}+\frac{480}{(\mu+\nu)\;(\mu+\nu+1)^9}\right]$$

$$(D|V|D'')_{NT} = +\,6!\,V_o\left[\frac{1344}{(\mu+\omega)^8(\mu+\omega+1)^4}+\frac{1920}{(\mu+\omega)^7(\mu+\omega+1)^5}+\frac{832}{(\mu+\omega)^6(\mu+\omega+1)^6}+\frac{-384}{(\mu+\omega)^5(\mu+\omega+1)^7}+\frac{0}{(\mu+\omega)^4(\mu+\omega+1)^8}+\frac{1408}{(\mu+\omega)^3(\mu+\omega+1)^9}+\frac{7488/5}{(\mu+\omega)^2(\mu+\omega+1)^{10}}\right]$$

$$(D'|V|D')_{NT} = -\,6!\,V_o\left[\frac{21/4}{\nu^9(2\nu+1)^2}+\frac{21/4}{\nu^8(2\nu+1)^3}+\frac{63/8}{\nu^7(2\nu+1)^4}\right.$$

$$+\frac{33/2}{\nu^6(2\nu+1)^5}+\frac{453/10}{\nu^5(2\nu+1)^6}+\frac{336/5}{\nu^4(2\nu+1)^7}$$

$$\left.+\frac{102/5}{\nu^3(2\nu+1)^8}+\frac{1304/5}{\nu^2(2\nu+1)^9}+\frac{5064/5}{\nu(2\nu+1)^{10}}\right]$$

$$(D'|V|D'')_{NT} = +\,6!\,V_o\left[\frac{10752}{(\nu+\omega)^9(\nu+\omega+1)^4}+\frac{10752}{(\nu+\omega)^8(\nu+\omega+1)^5}\right.$$

$$+\frac{8448}{(\nu+\omega)^7(\nu+\omega+1)^6}+\frac{5376}{(\nu+\omega)^6(\nu+\omega+1)^7}+\frac{-384/5}{(\nu+\omega)^5(\nu+\omega+1)^8}$$

$$\left.+\frac{1536/5}{(\nu+\omega)^4(\nu+\omega+1)^9}+\frac{51456/5}{(\nu+\omega)^3(\nu+\omega+1)^{10}}+\frac{12288}{(\nu+\omega)^2(\nu+\omega+1)^{11}}\right]$$

$$(D''|V|D'')_{NT} = -\,6!\,V_o\left[\frac{672}{\omega^9(2\omega+1)^6}+\frac{2016}{\omega^8(2\omega+1)^7}+\frac{1152}{\omega^7(2\omega+1)^8}\right.$$

$$\left.+\frac{-3840}{\omega^6(2\omega+1)^9}+\frac{-6912/5}{\omega^5(2\omega+1)^{10}}+\frac{27648}{\omega^4(2\omega+1)^{11}}+\frac{50688}{\omega^3(2\omega+1)^{12}}\right]$$

T_{13} potential elements:

$$(S|T_{13}|D) = -\frac{\Gamma V_0}{\tau}\left[\frac{4032/5}{(\lambda+\mu)^3(\lambda+\mu+\tau)^4} + \frac{8064/5}{(\lambda+\mu)^2(\lambda+\mu+\tau)^5} + \frac{1344}{(\lambda+\mu)\ (\lambda+\mu+\tau)^6}\right]$$

$$(S|T_{13}|D') = -\frac{\Gamma V_0}{\tau}\left[\frac{-25344}{(\lambda+\nu)^4(\lambda+\nu+\tau)^4} + \frac{-20736}{(\lambda+\nu)^3(\lambda+\nu+\tau)^5} + \frac{3840}{(\lambda+\nu)^2(\lambda+\nu+\tau)^6} + \frac{6912}{(\lambda+\nu)\ (\lambda+\nu+\tau)^7}\right]$$

$$(S|T_{13}|D'') = -\frac{\Gamma V_0}{\tau}\left[\frac{-23040}{(\lambda+\omega)^6(\lambda+\omega+\tau)^4} + \frac{-27648}{(\lambda+\omega)^5(\lambda+\omega+\tau)^5} + \frac{-4608}{(\lambda+\omega)^4(\lambda+\omega+\tau)^6} + \frac{18432}{(\lambda+\omega)^3(\lambda+\omega+\tau)^7} + \frac{16128}{(\lambda+\omega)^2(\lambda+\omega+\tau)^8}\right]$$

$$(D|T_{13}|D) = +\frac{\Gamma V_0}{\tau}\left[\frac{288}{\nu^5(2\nu+\tau)^4} + \frac{1152}{\nu^4(2\nu+\tau)^5} + \frac{27072/7}{\nu^3(2\nu+\tau)^6} + \frac{81792/7}{\nu^2(2\nu+\tau)^7} + \frac{21888}{\nu\ (2\nu+\tau)^8}\right]$$

$$(D|T_{13}|D') = -\frac{\Gamma V_0}{\tau}\left[\frac{-62208}{(\mu+\nu)^6(\mu+\nu+\tau)^4} + \frac{-87552}{(\mu+\nu)^5(\mu+\nu+\tau)^5} + \frac{50688/7}{(\mu+\nu)^4(\mu+\nu+\tau)^6} + \frac{48384}{(\mu+\nu)^3(\mu+\nu+\tau)^7} + \frac{-148608}{(\mu+\nu)^2(\mu+\nu+\tau)^8} + \frac{-299520}{(\mu+\nu)\ (\mu+\nu+\tau)^9}\right.$$

$$(D|T_{13}|D'') = 6!\,\frac{\Gamma V_o}{\tau}\left[\frac{9408/5}{(\mu+\omega)^8(\mu+\omega+\tau)^4} + \frac{2688}{(\mu+\omega)^7(\mu+\omega+\tau)^5} + \frac{13504/7}{(\mu+\omega)^6(\mu+\omega+\tau)^6} + \frac{3072/7}{(\mu+\omega)^5(\mu+\omega+\tau)^7} + \frac{-5184/5}{(\mu+\omega)^4(\mu+\omega+\tau)^8} + \frac{-9088/5}{(\mu+\omega)^3(\mu+\omega+\tau)^9} + \frac{-6336/5}{(\mu+\omega)^2(\mu+\omega+\tau)^{10}}\right]$$

$$(D'|T_{13}|D') = -\,\frac{\Gamma V_o}{\tau}\left[\frac{-3780}{\nu^7(2\nu+\tau)^4} + \frac{-7344}{\nu^6(2\nu+\tau)^5} + \frac{-179280/7}{\nu^5(2\nu+\tau)^6} + \frac{275211/14}{\nu^4(2\nu+\tau)^7} + \frac{104832}{\nu^3(2\nu+\tau)^8} + \frac{-117504}{\nu^2(2\nu+\tau)^9} + \frac{-1154304}{\nu(2\nu+\tau)^{10}}\right]$$

$$(D'|T_{13}|D'') = 6!\,\frac{\Gamma V_o}{\tau}\left[\frac{75264/5}{(\nu+\omega)^9(\nu+\omega+\tau)^4} + \frac{75264/5}{(\nu+\omega)^8(\nu+\omega+\tau)^5} + \frac{-3072}{(\nu+\omega)^7(\nu+\omega+\tau)^6} + \frac{-81408/7}{(\nu+\omega)^6(\nu+\omega+\tau)^7} + \frac{0}{(\nu+\omega)^5(\nu+\omega+\tau)^8} + \frac{44544/5}{(\nu+\omega)^4(\nu+\omega+\tau)^9} + \frac{-10752/5}{(\nu+\omega)^3(\nu+\omega+\tau)^{10}} + \frac{-10752}{(\nu+\omega)^2(\nu+\omega+\tau)^{11}}\right]$$

$$(D''|T_{13}|D'') = 6!\,\frac{\Gamma V_o}{\tau}\left[\frac{-336}{\omega^9(2\omega+\tau)^6} + \frac{-1008}{\omega^8(2\omega+\tau)^7} + \frac{-504}{\omega^7(2\omega+\tau)^8} + \frac{2496}{\omega^6(2\omega+\tau)^9} + \frac{2880}{\omega^5(2\omega+\tau)^{10}} + \frac{-9216}{\omega^4(2\omega+\tau)^{11}} + \frac{-21120}{\omega^3(2\omega+\tau)^{12}}\right]$$

T_{12} potential elements:

$$(D|T_{12}|D) = -6!\,\frac{\Gamma V_0}{\tau}\left[\frac{-7/5}{\mu^5(2\mu+\tau)^4}+\frac{-28/5}{\mu^4(2\mu+\tau)^5}+\frac{-12}{\mu^3(2\mu+\tau)^6}+\frac{-16}{\mu^2(2\mu+\tau)^7}+\frac{-56/5}{\mu(2\mu+\tau)^8}\right]$$

$$(D|T_{12}|D') = -6!\,\frac{\Gamma V_0}{\tau}\left[\frac{-448/5}{(\mu+\nu)^6(\mu+\nu+\tau)^4}+\frac{-896/5}{(\mu+\nu)^5(\mu+\nu+\tau)^5}+\frac{-1664/7}{(\mu+\nu)^4(\mu+\nu+\tau)^6}+\frac{-1856/7}{(\mu+\nu)^3(\mu+\nu+\tau)^7}+\frac{-1184/5}{(\mu+\nu)^2(\mu+\nu+\tau)^8}+\frac{-128}{(\mu+\nu)\;(\mu+\nu+\tau)^9}\right]$$

$$(D|T_{12}|D'') = -6!\,\frac{\Gamma V_0}{\tau}\left[\frac{256}{(\mu+\omega)^6(\mu+\omega+\tau)^6}+\frac{768}{(\mu+\omega)^5(\mu+\omega+\tau)^7}+\frac{1152}{(\mu+\omega)^4(\mu+\omega+\tau)^8}+\frac{1024}{(\mu+\omega)^3(\mu+\omega+\tau)^9}+\frac{2304/5}{(\mu+\omega)^2(\mu+\omega+\tau)^{10}}\right]$$

$$(D'|T_{12}|D') = -6!\,\frac{\Gamma V_0}{\tau}\left[\frac{-36/5}{\nu^7(2\nu+\tau)^4}+\frac{-144/5}{\nu^6(2\nu+\tau)^5}+\frac{-372/5}{\nu^5(2\nu+\tau)^6}+\frac{-792/5}{\nu^4(2\nu+\tau)^7}+\frac{-1552/5}{\nu^3(2\nu+\tau)^8}+\frac{-3008/5}{\nu^2(2\nu+\tau)^9}+\frac{-4128/5}{\nu(2\nu+\tau)^{10}}\right]$$

$$(D'|T_{12}|D'') = -6!\,\frac{\Gamma V_o}{\tau}\left[\frac{-7680/7}{(\nu+\omega)^7(\nu+\omega+\tau)^6} + \frac{-23040/7}{(\nu+\omega)^6(\nu+\omega+\tau)^7} + \frac{-20736/5}{(\nu+\omega)^5(\nu+\omega+\tau)^8} + \frac{-6144/5}{(\nu+\omega)^4(\nu+\omega+\tau)^9} + \frac{16896/5}{(\nu+\omega)^3(\nu+\omega+\tau)^{10}} + \frac{3072}{(\nu+\omega)^2(\nu+\omega+\tau)^{11}}\right]$$

$$(D''|T_{12}|D'') = -6!\,\frac{\Gamma V_o}{\tau}\left[\frac{144}{\omega^7(2\omega+\tau)^8} + \frac{1152}{\omega^6(2\omega+\tau)^9} + \frac{21888/5}{\omega^5(2\omega+\tau)^{10}} + \frac{9216}{\omega^4(2\omega+\tau)^{11}} + \frac{8448}{\omega^3(2\omega+\tau)^{12}}\right]$$

Appendix D

Units

Unit of energy: 8.33 Mev

Unit of length: $\frac{2.76 \times 10^{-13}}{2.33}$ cm.

The unit of energy was chosen to be a reasonable estimate of the binding energy of the triton.

The unit of length was chosen to be $r_o/2.33$, where r_o satisfies the equation

$$r_o \sqrt{\frac{M \epsilon_D}{\hbar^2}} = 0.64$$

M = mass of nucleon

ϵ_D = - B. E. of deuteron (2.23 Mev)

Appendix E

The Ritz Variational Method

One wishes to find an estimate of the lowest eigenvalue of a Hamiltonian H using a linear variation function

$$\psi = \sum_i A_i \psi_i$$

with the A's adjusted to obtain the lowest possible estimate of the energy E.

Inserting the trial function into the usual form of the variation principle, one obtains

$$E = \frac{\int \psi^* H \psi \, d\tau}{\int \psi^* \psi \, d\tau} = \frac{\int \sum A_i^* \psi_i^* \, H \sum A_j \psi_j \, d\tau}{\int \sum A_i^* \psi_i^* \sum A_j \psi_j \, d\tau}$$

$$= \frac{\sum_{ij} A_i^* H_{ij} A_j}{\sum_{ij} A_i^* \Delta_{ij} A_j}, \quad \text{where} \quad H_{ij} \equiv \int \psi_i^* H \psi_j \, d\tau, \quad \Delta_{ij} \equiv \int \psi_i^* \psi_j \, d\tau$$

which may be written as the equality:

$$\sum A_i^* E \Delta_{ij} A_j = \sum A_i^* H_{ij} A_j$$

If we differentiate both sides of this equality with respect to the various coefficients A_i^*, and impose the condition $\partial E/\partial A_i^* = 0$, thus assuring choice of optimum coefficients, we obtain a set of simultaneous equations

$$\sum_j (H_{ij} - E \Delta_{ij}) A_j = 0$$

which will possess a solution other than zero only if

$$\left| H_{ij} - E \Delta_{ij} \right| = 0$$

from which the lowest eigenvalue estimate and the associated transformation coefficients may be obtained.

The transformation coefficients, along with the normalization integrals, enable the computation of P_D, the percentage D state. The latter is defined in terms of a wave function

$$\psi = B_s \phi_s + B_D \phi_D ,$$

where ϕ_s and ϕ_D are the normalized S and D wave functions, by the expression

$$P_D = 100 \frac{(B_D)^2}{(B_s)^2 + (B_D)^2}$$

The expressions B_s and B_D may be evaluated at once by noting the identities

$$B_s \phi_s = A_s \psi_s$$

$$B_D \phi_D = A_D \psi_D + A_{D'} \psi_{D'} + A_{D''} \psi_{D''}$$

from which one may derive the relations, using the notation of the thesis,

$$(B_s)^2 = (S|S) \quad A_s^2$$

$$(B_D)^2 = A_D^2 (D|D) + A_{D'}^2 (D'|D') + A_{D''}^2 (D''|D'') + 2 A_D A_{D'} (D|D') + 2 A_D A_{D''} (D|D'') + 2 A_{D'} A_{D''} (D'|D'')$$

BIOGRAPHICAL NOTE

Robert Louis Pease was born in Fitchburg, Mass., on July 13, 1925. After education in the public schools of Hamilton, Ontario (Canada), Toledo, Ohio, and Hamilton, Ohio, he entered Miami University, Oxford, Ohio, in 1940 and received his A. B. in August, 1943.

Following a brief period as instructor in physics at Miami, he entered the Massachusetts Institute of Technology as graduate student and teaching fellow. He transferred to the Radiation Laboratory as a staff member in March, 1944, but left shortly thereafter to serve as an electronics officer in the United States Naval Reserve.

In the fall of 1946, he re-entered the Institute as graduate student and teaching fellow. During the academic year 1948-9 he held the E. I. duPont de Nemours Fellowship in Physics; he is at present the holder of an Atomic Energy Commission Fellowship.

He is a member of Phi Beta Kappa, Phi Eta Sigma, Sigma Pi Sigma, Sigma Xi, and the American Physical Society.