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Normal States of Nuclear Three- and Four-Body Systems

HENRY MARGENAU AND DANA T. WARREN
Sloane Physics Laboratory, Yale University, New Haven, Connecticut

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A variational method employing orthogonal (Hermite) functions in linear combination is used for calculating the binding energies of H^3 and He^4, with the following choice of nuclear constants:

$$A = 35.60 \text{ Mev}; \quad a = 2.25 \times 10^{-13} \text{ cm}; \quad g = 0.20,$$

and an error function potential. Two types of coordinates are used for H^3; (1) normal, (2) individual particle coordinates. Their advantages and disadvantages are discussed. With the use of a certain limited set of functions of normal coordinates the energy has been depressed from −6.21 Mev in zeroth approximation to −7.21 Mev, while a suitable set of functions involving only individual particle coordinates reduced it from −6.16 Mev to −6.84 Mev. The second Schrödinger perturbation is less effective than the latter scheme by 0.22 Mev. Functions of different symmetry, called into play by the Heisenberg operators, are found to contribute 0.07 Mev on the basis of a modified variation method. He^4 has been treated only with the use of individual particle coordinates (Hartree method). A similar group of functions lowers the energy from −24.81 Mev in zeroth approximation to −25.85 Mev, which is better than the effect of Schrödinger's perturbation theory by 0.25 Mev. General estimates of convergence limits are given.

THE theory of nuclear forces appears to have reached a stage in which it allows most of the details in the interaction of nuclear particles to be understood in a reasonably quantitative manner, so that there can be but little doubt as to its essential correctness. The chief obstacle in the way of exact formulations lies in the mathematical difficulties surrounding the quantum-mechanical many-body problem. These obstacles are bound to become more serious as theories become more refined. It is in an attempt at understanding the limitations of the various methods designed to treat the three- and four-body problems, if not at the partial removal of these limitations, that the present calculations were undertaken.

The list of papers which deal with applications of the variational method to the problem at hand, starting with the publications of Wigner[1] and of Feenberg,[2] is already long. In the papers just mentioned an elegant and simple scheme for estimating the energy of the lowest state of many-body systems, known as the "equivalent two-body method," has been designed, a scheme which has proved very useful in the evaluation of probably universal nuclear constants.[3] It is clearly desirable to provide as refined as possible a variational basis for the use of the equivalent two-body method, an objective which has inspired the work to be described. We feel that the results are such as to strengthen confidence in the abbreviated two-body procedure.

The most adequate and extensive variational calculations have been applied to the three-body problem by Present,[4] and by Rarita and Present.[5] Their method, while probably superior to the one here developed in several points—particularly the rapidity of convergence—has the serious disadvantage of being very difficult to apply to more than three particles. It seems important, however, to have a method which permits application without change in principle to any number of particles, and it is perhaps a further point in favor of the present line of attack that it starts with Feenberg's[2] elementary procedure as a first approximation. Rarita and Present[5] reach the conclusion that the values of nuclear parameters which will yield correctly the mass defect of H^3, while satisfying experimental data of neutron-proton scattering and the mass defect of H^2, give too large a binding energy for He^4. This result stimulates reinvestigation by another method. In our work we find, employing the usual values of nuclear parameters, an apparent convergence of the energy of H^3 to −7.21 Mev, 1 Mev above the experimental value. If this value were near the true convergence limit, the present results would support the conclusions of

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[1] E. Wigner, Phys. Rev. **43**, 252 (1933).

[2] E. Feenberg, Phys. Rev. **47**, 850 (1935).

[3] E. Feenberg and J. K. Knipp, Phys. Rev. **48**, 906 (1935).

[4] R. D. Present, Phys. Rev. **50**, 635 (1936).

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

Rarita and Present and require considerable revision of the present theories. On the other hand we know, from an application of the methods of this paper to H^2, that there occurs a similar semblance of convergence toward an energy value which is not at all near the true energy, if an analogous, limited set of functions is used. Because of this circumstance we suggest that there may be no necessity for seriously questioning the usual values of nuclear parameters.

Schrödinger perturbation theory has been applied to light nuclei by Inglis.[6] Nothing is known with certainty about the convergence of this method for nuclei, and the best way to test it is to make a variational calculation with the same functions as those used in the perturbation scheme. This was done for He^4, and it was found that the two methods do not differ very much in their results, the present method being slightly better. Such a coincidence is not trivial or in general predictable. While it might be expected in cases where the variation functions approximate the correct ones reasonably well, so that the unperturbed eigenvalues are nearly equal to the diagonal elements of the correct operator, it is somewhat of an accident in the nuclear problem; for here the oscillator eigenvalues employed by Inglis are often quite different from the corresponding H_{ii} which enter in the variational calculation, sometimes by 100 percent. The coincidence is therefore not without interest. For H^3 the variation method also gives, with the use of the same functions, a slightly lower energy than the perturbation theory, as will be shown.

I. Outline of Method

The simple variation functions of the Gauss type in relative coordinates, used by Feenberg[2] and by Bethe and Bacher[7] represent the lowest member of a complete set of functions, the Hermite orthogonal functions. It is therefore natural to inquire what the effect of an inclusion of the higher members of this set will be. Since all these functions have the wrong asymptotic behavior one might expect the convergence to the energy limit to be none too rapid, and a special investigation of this point is necessary. This we have carried out by applying the method to the case of the deuteron where the correct limit is known. The results, together with certain findings regarding the use of different types of coordinates and their adequacy for nuclear calculations, will be published in a subsequent paper.

Having once chosen n orthogonal and normal functions in a suitable set of coordinates, and having ascertained the correct form of the Hamiltonian operator H in these coordinates, the problem of calculating the lowest energy reduces to solving the determinantal equation $|H_{ij}-\delta_{ij}E|=0$ for E. This process is simplified if we are interested only in the lowest of the n roots, which, for the nuclear problem, is widely separated from the next higher one. For we may then write for E the difference $H_{00}-\Delta E$ and introduce an estimated value of ΔE in all diagonal elements except the one involving H_{00}, which becomes ΔE. We write this element in the lower right-hand corner of the determinant and reduce the latter numerically by adding the first row with a suitable factor to all other rows so as to put zeros in the first column. Every single application of this process adds a negative increment to ΔE, and after an $(n-1)$-fold application the equation reads $\Delta E-\epsilon=0$. If ϵ is not sufficiently close to the original estimate the reduction is repeated with the new value. In the cases we have chosen the process is quite insensitive and highly stable with respect to the original choice of ΔE, and it is not very time consuming, even with as many as 20 linear variation functions. Most of the work is involved in the calculation of the elements H_{ij}. This, however, was found somewhat laborious and has forced us to use a single fixed form for the interaction between nuclear particles, symmetric in all of them, *viz.*

$$U_{ij}=-Ae^{-r^2_{ij}/a^2}[(1-g)P_{ij}^M+gP_{ij}^H], \quad (1)$$

where the symbols have the usual significance.[3] The parameters were chosen so as to make the binding energy of H^2 equal to 2.15 Mev, to give very approximately the experimental binding energies of H^3, He^4 with the use of the equivalent two-body method, and to be consistent with

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[6] D. R. Inglis, Phys. Rev. **51**, 531 (1937).

[7] H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8**, 82 (1936).

scattering data,[8] as follows:

$$A=35.60 \text{ Mev.},\quad a=2.25\times 10^{-13} \text{ cm},\quad g=0.20.$$

The Coulomb energy, which according to previous calculations affects the total energy but slightly, will be omitted from the variational calculation on He^4 for convenience and added in afterwards. We shall also neglect for the present the effect upon the lowest state of functions unsymmetrical in like particles, which should properly be included because of the term $P_{ij}{}^H$ in (1); their effect is also known to be small.[9] (Cf. Section II, C.) If thus we limit ourselves to functions which are completely symmetrical in like particles, assumption (1) leads to the following form[10] for the Hamiltonian operator, written in central, individual particle coordinates:

$$H=\frac{\hbar^2}{2M}\sum_i \Delta_i{}^2-B\sum_{ij}{}_1 \exp\left[-(\mathbf{r}_i-\mathbf{r}_j)^2/a^2\right]P_{ij}$$
$$-C\sum_{ij}{}_2 \exp\left[-(\mathbf{r}_i-\mathbf{r}_j)^2/a^2\right]P_{ij} \quad (2)$$

where Σ_1 is extended over pairs of unlike, Σ_2 over pairs of like particles. $B=(1-\frac{1}{2}g)A=32.10$ Mev; $C=(1-2g)A=21.77$ Mev; P_{ij} simply permutes the position coordinates of the ith and jth particles.

As to the choice of variation functions, the general rule is that they should at once be combined so as to possess the same symmetry in the various particles as does (2). This reduces the number of independent functions and hence the labor in reducing the determinant. Furthermore it is usually unnecessary to include functions which do not combine directly with the one corresponding to the lowest energy, for their contribution was found in most cases to be of secondary magnitude. Elimination of a function may sometimes be made by trial and error, using the function alone in combination with the "lowest" one; but this procedure is not always safe because a function, while feeble alone, may gain power in collaboration with others. Finally, as one would gather from the symmetry of (2) with respect to the three Cartesian axes, the best function for the lowest states of H^3 and He^4, neither of which has orbital space degeneracy, is one which is symmetrized in x, y, and z. Hence this procedure is carried out on all trial functions.

All the present work involves simple harmonic oscillator functions; it is related in this respect to the investigations of Houston,[11] and Heisenberg.[12] We shall use the following notation: Single Hermite functions will be denoted by

$$\varphi_n(x)=N_n e^{-x^2/2}H_n(x), \quad (3)$$

where N_n is a normalizing factor and H_n a Hermite polynomial. We define further

$$\varphi_{lmn}(i)=\varphi_l(x_i)\varphi_m(y_i)\varphi_n(z_i) \quad (4)$$

and

$$\Phi_{lmn}=(1/6)^{\frac{1}{2}}(1+\delta_{lm}+\delta_{ln}+\delta_{mn}+2\delta_{lm}\delta_{ln}\delta_{mn})^{-\frac{1}{2}}$$
$$\times(\varphi_{lmn}+\varphi_{lnm}+\varphi_{mln}+\varphi_{mnl}+\varphi_{nlm}+\varphi_{nml}). \quad (5)$$

Eq. (5) is merely a compact way of writing the result of symmetrizing a function like (4) with the correct normalizing factor.

II. VARIATION METHOD APPLIED TO H^3

A. Use of relative coordinates

The Hamiltonian for the H^3 problem reads (the index 1 here refers to the proton)

$$H=-(\hbar^2/2M)(\nabla_1{}^2+\nabla_2{}^2+\nabla_3{}^2)$$
$$-B\exp\left[-r_{12}{}^2/a^2\right]P_{12}$$
$$-B\exp\left[-r_{13}{}^2/a^2\right]P_{13}$$
$$-C\exp\left[-r_{23}{}^2/a^2\right]P_{23}.$$

The transformation to relative and center of mass coordinates,

$$\xi_1=(1/2)^{\frac{1}{2}}(2x_1-x_2-x_3),\quad \xi_2=(1/2)^{\frac{1}{2}}(x_2-x_3),$$
$$X=(1/3)^{\frac{1}{2}}(x_1+x_2+x_3)_y$$

with similar relations between η and y, ρ and z, changes the form of H into

$$H=-(\hbar^2/2M)(\nabla^2+3\nabla_1{}^2+\nabla_2{}^2)$$
$$-B\exp\left[-(\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_2)^2/2a^2\right]P_{12}$$
$$-B\exp\left[-(\boldsymbol{\varrho}_1+\boldsymbol{\varrho}_2)^2/2a^2\right]P_{13}$$
$$-C\exp\left[-2\rho_2{}^2/a^2\right]P_{23},$$

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[8] G. Breit, E. U. Condon, and R. D. Present, Phys. Rev. **50**, 825 (1936); M. A. Tuve, N. P. Heidenburg, and L. R. Hafstad, Phys. Rev. **50**, 806 (1936).

[9] G. Breit and E. Feenberg, Phys. Rev. **50**, 850 (1936); R. D. Present, Phys. Rev. **50**, 870 (1936).

[10] Cf. for instance Bethe and Bacher, reference 7.

[11] W. V. Houston, Phys. Rev. **47**, 942 (1935).

[12] W. Heisenberg, Zeits. f. Physik **96**, 473 (1935).

where $\rho^2=\xi^2+\eta^2+\zeta^2$. It allows us to separate off the motion of the center of mass, ∇^2, but we pay for this advantage by having to use more complicated P-operators. They become linear substitutions:

$$\begin{aligned} &P_{12}\xi_1=\tfrac{1}{2}(-\xi_1+3\xi_2) && P_{12}\xi_2=\tfrac{1}{2}(\xi_1+\xi_2) \\ &P_{13}\xi_1=-\tfrac{1}{2}(\xi_1+3\xi_2) && P_{13}\xi_2=-\tfrac{1}{2}(\xi_1-\xi_2) \\ &P_{23}\xi_1=\xi_1 && P_{23}\xi_2=-\xi_2 \end{aligned} \tag{6}$$

with similar relations for η and ζ. This complication, of course, accompanies the transition from individual particle coordinates to any new set which corresponds to the correct number of degrees of freedom. We note that the function

$$\begin{aligned}\psi=\varphi_{n_{\xi_1}}(q_1^{\frac{1}{2}}\xi_1)\varphi_{n_{\eta_1}}(q_1^{\frac{1}{2}}\eta_1)\varphi_{n_{\zeta_1}}(q_1^{\frac{1}{2}}\rho_1)\varphi_{n_{\zeta_2}}(q_2^{\frac{1}{2}}\xi_2)\\ \times\varphi_{n_{\eta_2}}(q_2^{\frac{1}{2}}\eta_2)\varphi_{n_{\zeta_2}}(q_2^{\frac{1}{2}}\rho_2)\end{aligned} \tag{7}$$

satisfies the equation

$$(\hbar^2/2M)\{-(3\nabla_1^2+\nabla_2^2)+(3q_1^2\rho_1^2+q_2^2\rho_2^2)\}\psi=E\psi$$

and has the eigenvalue

$$\begin{aligned}E(n_{\xi 1}\cdots n_{\zeta 2})=(\hbar^2/M)[(n_{\xi 1}+n_{\eta 1}+n_{\zeta 1}+3/2)3q_1\\ +(n_{\xi 2}+n_{\eta 2}+n_{\zeta 2}+3/2)q_2].\end{aligned}$$

If, therefore, we use functions of the type (7) the kinetic energy is easily calculated from the relation

$$\begin{aligned}-(\hbar^2/2M)(3\nabla_1^2+\nabla_2^2)\psi=E(n_{\xi 1}\cdots n_{\zeta 2})\psi\\ -(\hbar^2/2M)(3q_1^2\rho_1^2+q_2^2\rho_2^2)\psi.\end{aligned} \tag{8}$$

In setting up variation functions we have at our disposal not only the coefficients with which functions (7) enter into linear combination, but also the parameters q_1 and q_2. These must be fixed before the coefficients can be determined. The plausible thing to do in this connection is to choose q_1 and q_2 so that the "lowest" function minimizes the energy, as was also done by Inglis.[6] We have checked this method with some care for H^2 and found that the final energy varies with q in nearly the same manner as H_{00} over a surprisingly large range.[14]

The zero-order function of the set (7) is, if written explicitly,

$$\begin{aligned}\psi_0&=\exp[-q_1\rho_1^2/2-q_2\rho_2^2/2]\\ &=\exp[-q_1(r_{12}^2+r_{13}^2+2\mathbf{r}_{12}\cdot\mathbf{r}_{23})/4-q_2r_{23}^2/4].\end{aligned}$$

It differs from the one employed by Feenberg[2] and by Bethe and Bacher[7] by having the product term in the exponent. As far as the minimization of H is concerned, however, this term is indifferent; for while the expression for $\int\psi_0H\psi_0d\tau$, in terms of q_1 and q_2 looks different, the substitutions

$$p=4q_2/(9q_1+q_2),\quad \sigma=(9q_1+q_2)a^2/8$$

reduce it to the same form as that given by Bethe and Bacher, Eq. (118). The minimum E_0 is therefore the same except for the slight difference in the parameters. Its value is -6.21 Mev, it occurs for $q_1=0.1263$, $q_2=0.3394$.

Calculations were carried out chiefly with the following functions:

$$\begin{aligned} &\psi_0=\Phi_{000}(1)\Phi_{000}(2), && \psi_7=\Phi_{000}(1)\Phi_{400}(2),\\ &\psi_2=\Phi_{110}(1)\Phi_{110}(2), && \psi_8=\Phi_{400}(1)\Phi_{000}(2),\\ &\psi_2=\Phi_{200}(1)\Phi_{000}(2), && \psi_9=\Phi_{200}(1)\Phi_{400}(2),\\ &\psi_3=\Phi_{000}(1)\Phi_{200}(2), && \psi_{10}=\Phi_{400}(1)\Phi_{200}(2),\\ &\psi_4=\Phi_{200}(1)\Phi_{200}(2), && \psi_{11}=\Phi_{220}(1)\Phi_{220}(2),\\ &\psi_5=\Phi_{220}(1)\Phi_{000}(2), && \psi_{12}=\Phi_{400}(1)\Phi_{400}(2).\\ &\psi_6=\Phi_{000}(1)\Phi_{220}(2), && \end{aligned} \tag{9}$$

The effect of the functions having quantum numbers (112)(110); (310)(110); (220)(200); (400)(220) has also been considered and found to be small.

If i and j refer to two functions of this set, and q_1 and q_2 are given the above values, the matrix elements are, in view of (8),[13]

$$\begin{aligned}H_{ij}=E_i\delta_{ij}-(S_{ij}+T_{ij}+U_{ij}+7.770(q_1\rho_1^2)_{ij}\\ +6.958(q_2\rho_2^2)_{ij})\end{aligned} \tag{10}$$

$(q_1\rho_1^2)_{ij}$ and $(q_2\rho_2^2)_{ij}$ are pure numbers, at once expressible in terms of oscillator matrix elements:

$$(\xi^2)_{n,\,n}=n+\tfrac{1}{2},\quad (\xi)^2_{n,\,n+2}=\tfrac{1}{2}[(n+1)(n+2)]^{\frac{1}{2}}.$$

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[13] Energies are expressed throughout in Mev, and the unit of length is 10^{-13} cm, as in reference 7.

Furthermore,

$$S_{ij}=B\int \psi_i \exp\left[-(\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_2)^2/2a^2\right]P_{12}\psi_j d\tau,$$

$$T_{ij}=B\int \psi_i \exp\left[-(\boldsymbol{\varrho}_1+\boldsymbol{\varrho}_2)^2/2a^2\right]P_{13}\psi_j d\tau,$$

$$U_{ij}=C\int \psi_i \exp\left[-2\rho_2^2/a^2\right]P_{23}\psi_j d\tau.$$

S_{ij} splits up into sums of terms, each of which is a product of three integrals of the type

$$S_{kl;\,mn}=N_{klmn}\int\int H_k(q_1^{\frac{1}{2}}\xi_1)H_l(q_2^{\frac{1}{2}}\xi_2)$$
$$\times\exp\left[(-q_1+1/2a^2)\xi_1^2-(q_2+1/2a^2)\xi_2^2\right.$$
$$\left.+\xi_1\xi_2/a^2\right]H_m(q_1^{\frac{1}{2}}P_{12}\xi_1)H_n(q_2^{\frac{1}{2}}P_{12}\xi_2)d\xi_1 d\xi_2.$$

The algebraic expressions for the s integrals are lengthy and will not be given. As a consequence of the symmetry of the Hamiltonian the T_{ij} terms are related to the S_{ij} and need not be calculated separately. T differs from S only by an application of P_{23} to the factor $\exp\left[-(\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_2)^2/2a^2\right]$ in the integrand. But P_{23} may be applied to the whole integrand without changing the value of the integral. P_{23}, however, affects only the variable ρ_2, changing its sign. Hence the passage from S to T changes the sign of the integral if the integrand is odd in ρ_2, leaves it unchanged if it is even. We see, therefore, that

$$T_{ij}=\pm S_{ij},$$

the upper sign holding when ψ_i and ψ_j are both even or both odd in ξ_2. U_{ij} is easier to calculate because P_{23} causes no mixing of the coordinates. It is zero unless ψ_i and ψ_j contain the same function of $\boldsymbol{\varrho}_1$.

The result of the variational calculations is best seen from Table I. The functions are labeled in accordance with (9). The functions indicated below that list have also been considered and found to lower the energy by as much as 0.08 Mev if combined with certain others, but if they are included together with $\psi_0-\psi_{12}$ their effect is inappreciable. It is clear that the chief contribution comes from the quadruply excited states, a result which agrees with the calculations of Inglis, using perturbation theory.

It has seemed too laborious a task to introduce all the octuply excited functions. What, then, may we say about convergence at the present stage? There is certainly a semblance of convergence toward the value -7.21 Mev. Nevertheless experience with the deuteron problem[14] has taught us that a similar group of functions, employed in the same way, leaves about half a megavolt of binding energy unaccounted for, and that, when it is difficult to get beyond a certain energy value, that value may not be the limit. On the other hand the variation functions for H^3 are more concentrated than those for H^2, which implies that the present method will reach the limit somewhat faster. Taking account of these considerations and realizing that the error for H^3 with similar functions of the same degree of concentration is probably somewhat larger than for H^2, we believe the true limit of the present scheme to lie at about -7.7 Mev. The true theoretical binding energy with the interaction parameters here chosen would be slightly below this value since the mixing effect[9] due to Heisenberg forces and relativity corrections[15] have here been neglected. The equivalent two-body method gives approximately the experimental value -8.3 Mev with the present parameters.

B. Use of individual particle coordinates

When applied to more particles, the method outlined so far becomes unwieldy because of the complicated nature of the permutation operators. Recourse is therefore often had to functions of individual particle coordinates in analogy with Hartree's atomic method. It seemed of interest to investigate in connection with the simple example of H^3 the relative merits of the two procedures.

TABLE I. *Variational energies of H^3 for different combinations of functions in normal coordinates.*

FUNCTIONS INCLUDED	$-E$(Mev)
ψ_0	6.214
ψ_0, ψ_1	6.243
$\psi_0-\psi_3$	6.244
$\psi_0-\psi_3$, ψ_5	6.39
ψ_0, $\psi_4-\psi_8$	7.11
$\psi_0-\psi_9$	7.21
$\psi_0-\psi_{12}$	7.21

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[14] The results will be published shortly.

[15] D. Blochinzew, Physik. Zeits. Sowjetunion **8**, 270 (1935); H. Margenau, Phys. Rev. **50**, 342 (1936); E. Feenberg, Phys. Rev. **50**, 674 (1936).

Hartree functions describing the state of a nucleus include the motion of the center of mass, and this must be subtracted operationally from the Hamiltonian. The term to be subtracted from the usual H is the kinetic energy of the center of mass which, for N particles all of the same mass M, has the form

$$-(\hbar^2/2NM)(\sum_i \nabla_i)^2$$

Thus we have left as the significant Hamiltonian to be used in the variational problem[6]

$$H=-(\hbar^2/2M)[(1-1/N)\sum_i \nabla_i^2 \\ -2/N\sum_{i>j}\nabla_i\cdot\nabla_j]+E_{\text{pot}}. \quad (11)$$

For H^3 we have

$$H=-(\hbar^2/3M)[\sum_i \nabla_i^2-\sum_{i>j}\nabla_i\cdot\nabla_j] \\ -B\exp[-r_{12}^2/a^2]P_{12}-B\exp[-r_{13}^2/a^2]P_{13} \\ -C\exp[-r_{23}^2/a^2]P_{23}. \quad (12)$$

We have employed the following 21 normalized variation functions:

$$\begin{array}{c|c|c}
\phi_{000}(1)\phi_{000}(2)\phi_{000}(3)=\psi_0 & \phi_{000}(1)\phi_{200}(2)\phi_{200}(3) & \phi_{200}(1)\phi_{100}(2)\phi_{100}(3) \\
(1/2)^{\frac{1}{2}}\phi_{000}(1)[\phi_{200}(2)\phi_{000}(3)+] & (1/2)^{\frac{1}{2}}\phi_{200}(1)[\phi_{200}(2)\phi_{000}(3)+] & (1/2)^{\frac{1}{2}}\phi_{100}(1)[\phi_{200}(2)\phi_{100}(3)+] \\
\phi_{200}(1)\phi_{000}(2)\phi_{000}(3) & (1/2)^{\frac{1}{2}}\phi_{000}(1)[\phi_{100}(2)\phi_{300}(3)+] & (1/2)^{\frac{1}{2}}\phi_{000}(1)[\phi_{220}(2)\phi_{000}(3)+] \\
\phi_{000}(1)\phi_{100}(2)\phi_{100}(3) & (1/2)^{\frac{1}{2}}\phi_{300}(1)[\phi_{100}(2)\phi_{000}(3)+] & \phi_{220}(1)\phi_{000}(2)\phi_{000}(3) \\
(1/2)^{\frac{1}{2}}\phi_{100}(1)[\phi_{000}(2)\phi_{100}(3)+] & (1/2)^{\frac{1}{2}}\phi_{100}(1)[\phi_{300}(2)\phi_{000}(3)+] & (1/2)^{\frac{1}{2}}\phi_{000}(1)[\phi_{120}(2)\phi_{100}(3)+] \\
(1/2)^{\frac{1}{2}}\phi_{000}(1)[\phi_{400}(2)\phi_{000}(3)+] & \phi_{000}(1)\phi_{110}(2)\phi_{110}(3) & (1/2)^{\frac{1}{2}}\phi_{100}(1)[\phi_{000}(2)\phi_{120}(3)+] \\
\phi_{400}(1)\phi_{000}(2)\phi_{000}(3) & (1/2)^{\frac{1}{2}}\phi_{110}(1)[\phi_{110}(2)\phi_{000}(3)+] & (1/2)^{\frac{1}{2}}\phi_{120}(1)[\phi_{000}(2)\phi_{100}(3)+].
\end{array} \quad (13)$$

A plus sign indicates that a function similar to the foregoing one, but with particles 2 and 3 interchanged, has been added. (13) represents oscillator eigenfunctions for a potential energy

$$(\hbar^2/2M)q^2(r_1^2+r_2^2+r_3^2),$$

that is, the oscillator "stiffness" is taken to be equal for all particles. We are thus at once disposing of possible variation parameters whose retention would, however, give only a very slight improvement. q appears of course in the functions (13). To allow comparison with the work of Inglis[6] we introduce the dimensionless quantity $\sigma\equiv qa^2$.

As before, we fix σ by minimizing H_{00}. The minimum occurs at $\sigma=1.83$ and has the value -6.16 Mev. This compares not unfavorably with the value -6.21 Mev obtained in the previous section for H_{00} with the use of two parameters. Expressing again the energy in Mev and distances in units of 10^{-13} cm, we find in this instance

$$H_{ij}=2/3E_i\delta_{ij}-4.945/(3)[(\sum qr^2)_{ij} \\ -(\sum_{n>m}\nabla_n\cdot\nabla_m)_{ij}/q]-2S_{ij}-U_{ij}.$$

$E_i=(\hbar^2/M)q(9/2+\Sigma n_i)=14.83(9/2+\Sigma n_i)$, where the n_i are the quantum numbers of state i. The matrix elements are written so that the terms in parentheses are pure numbers. The expression $(\sum_{n>m}\nabla_n\cdot\nabla_m/q)_{ij}$ at once decomposes into products of two integrals of the form

$$d_{st}=\int_{-\infty}^{\infty}\varphi_s(x)\frac{d}{dx}\varphi_t(x)dx=\left(\frac{s+1}{2}\right)^{\frac{1}{2}}\delta_{t,\,s+1}.$$

Since the functions chosen are symmetrical in particles 2 and 3, the integrals over the two terms of (12) involving B are equal, and P_{23} may be ignored. This makes the integrations very easy. All S_{ij} and T_{ij} reduce to products of integrals

$$f_{kl,\,mn}=\left(\frac{\sigma+2}{\sigma}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}H_k(\xi_1)H_l(\xi_2) \\ \times\exp\{-[\xi_1^2+\xi_2^2+(\xi_1-\xi_2)^2/\sigma]\} \\ \times H_m(\xi_1)H_n(\xi_2)d\xi_1 d\xi_2,$$

many of which have already been given by Inglis. These f's are polynomials in the quantity

$$u=1/(\sigma+2).$$

The coefficients of the various powers of u for the integrals needed in this work are tabulated in Table II, where no entry indicates a zero.

After calculation of the H_{ij}, the secular determinant, which now has 21 rows and columns, was reduced as explained before. The effect of simpler combinations among the functions was not studied in as much detail as in the previous section, the results being somewhat parallel to that case. The 20 functions here considered in addition to ψ_0 lower the energy from -6.16 Mev to -6.84 Mev. It is seen that the Hartree method is distinctly poorer than the one employed in II, A.

If the same functions are used with the Schrödinger perturbation method it is found that the second perturbation depresses the energy from -6.16 Mev to -6.62 Mev.

C. Effect of Heisenberg operators

Although previous calculations[9] show that the depressing effect of an antisymmetrical function in the position coordinates of the two neutrons upon the energy of the normal state is small, we have made a careful study of this matter for the case of H^3, using what is essentially a variation method.

We wish to satisfy the equation

$$H\psi = E\psi,$$

in which[14]

$$H = T + U_{12} + U_{13} + U_{23}.$$

T denotes the kinetic energy as it appears explicitly in (11) (we shall use "Hartree functions" in this section), and the U's are defined in Eq. (1). If we let

$$\psi = auS^0 + bvS^1, \tag{15}$$

where S^0 and S^1 are the spin functions used by Breit and Feenberg,[9] u is symmetrical and v antisymmetrical in particles 2 and 3, and a and b are normalizing factors,[16] then the orthogonality of S^0 and S^1 will cause (14) to reduce to two equations:

$$\left.\begin{aligned} H_0au + Xbv &= Eau \\ H_1bv + Xau &= Ebv \end{aligned}\right\} \begin{aligned} &\text{(a)} \\ &\text{(b)} \end{aligned} \tag{16}$$

where H_0 is the Hamiltonian (11) which was previously used,

$$X = (3^{\frac{1}{2}}/2)g(J_{13}P_{13} - J_{12}P_{12}),$$

$$J_{ij} = -A \exp\left[-r_{ij}^2/a^2\right]$$

and

$$H_1 = T - J_{23} + (1 - 3g/2)(J_{13}P_{13} + J_{12}P_{12}). \tag{17}$$

Let us put

$$E_1 = \int vH_1vd\tau. \tag{18}$$

We have already found an approximation to

$$E_0 = \int uH_0ud\tau.$$

TABLE II. *Numerical coefficients occurring in f-integrals (individual particle coordinates).*

	1	u	u^2	u^3	u^4
$f_{00,\,00}$	1				
$f_{11,\,00}$		1			
$f_{10,\,10}$	1	-1			
$f_{20,\,00}$		$-(1/2)^{\frac{1}{2}}$			
$f_{11,\,11}$	1	-2	3		
$2^{\frac{1}{2}}f_{21,\,10}$		2	-3		
$2^{\frac{1}{2}}f_{21,\,01}$		-1	3		
$f_{20,\,20}$	1	-2	$3/2$		
$f_{22,\,00}$			$3/2$		
$f_{31,\,00}$			$-(3/2)^{\frac{1}{2}}$		
$(2/3)^{\frac{1}{2}}f_{30,\,10}$		-1	1		
$f_{40,\,00}$			$(3/8)^{\frac{1}{2}}$		
$f_{21,\,21}$	1	-3	$15/2$	$-15/2$	
$f_{22,\,11}$		2	-6	$15/2$	
$2^{\frac{1}{2}}f_{22,\,20}$		-1	6	$-15/2$	
$(2/3)^{\frac{1}{2}}f_{31,\,11}$		-1	4	-5	
$(1/3)^{\frac{1}{2}}f_{32,\,10}$			$3/2$	$-5/2$	
$(1/3)^{\frac{1}{2}}f_{32,\,01}$			-1	$5/2$	
$(1/3)^{\frac{1}{2}}f_{31,\,20}$		1	-3	$5/2$	
$f_{33,\,00}$				$5/2$	
$f_{30,\,30}$	1	-3	$9/2$	$-5/2$	
$(2/3)^{\frac{1}{2}}f_{41,\,10}$			-2	$5/2$	
$(2/3)^{\frac{1}{2}}f_{41,\,01}$			$1/2$	$-5/2$	
$(1/3)^{\frac{1}{2}}f_{42,\,00}$				$-5/4$	
$(1/3)^{\frac{1}{2}}f_{40,\,20}$		-1	2	$-5/4$	
$f_{22,\,22}$	1	-4	15	-30	$105/4$
$(2/3)^{\frac{1}{2}}f_{32,\,21}$		2	-9	20	$-35/2$
$f_{33,\,11}$			$9/2$	-15	$35/2$
$f_{31,\,31}$	1	-4	$27/2$	-25	$35/2$
$(2/3)^{\frac{1}{2}}f_{42,\,20}$			$9/2$	-15	$105/8$
$f_{43,\,10}$				5	$-35/4$
$f_{41,\,30}$		2	-9	15	$-35/4$
$f_{44,\,00}$					$35/8$
$f_{40,\,40}$	1	-4	9	-10	$35/8$

---

[16] u and v are assumed normalized.

If now we multiply 16 (a) and (b) by u and v, respectively, and integrate, we obtain

$$\left.\begin{aligned} E&=E_0+(b/a)\int uXvd\tau \quad &\text{(a)}\\ E&=E_1+(a/b)\int vXud\tau \quad &\text{(b)}\end{aligned}\right\} \tag{19}$$

The two integrals appearing here are equal and will be denoted by

$$s=\int uXvd\tau. \tag{20}$$

b/a may be eliminated from 19 (a) and (b), so that the result will be

$$E=E_0+\tfrac{1}{2}\{E_1-E_0\pm[(E_1-E_0)^2+4s^2]^{\frac{1}{2}}\}. \tag{21}$$

To make this as small as possible the negative sign must be chosen. For small s this equation reduces to

$$E=E_0-s^2/(E_1-E_0),$$

which is essentially the result of Breit and Feenberg in a form in which it shows more clearly the meaning of E_1.

Both E_1 and s depend upon the choice of the antisymmetrical function v. The procedure now is to select a somewhat flexible v, to calculate E_1 and s according to (18) and (20), and to find the lowest value of (21). Two types of function were tried. The first was

$$v=(1/2)^{\frac{1}{2}}\phi_{000}(1)[\phi_{200}(2)\phi_{000}(3)-\phi_{000}(2)\phi_{200}(3)]$$

with a variable stiffness q in the oscillator functions. This gave somewhat poorer results than the second choice

$$v=c(J_{13}-J_{12})\psi_0(\sigma'). \tag{22}$$

$\psi_0(\sigma')$ is the function appearing in the list (13), but with a variable parameter σ' which need not be the same as σ. The normalizing constant turns out to be

$$c=2^{-\frac{1}{2}}A^{-1}\left[\left(\frac{\sigma'}{\sigma'+4}\right)^{\frac{3}{2}}-\left(\frac{\sigma'}{\sigma'+1}\cdot\frac{\sigma'}{\sigma'+3}\right)^{\frac{3}{2}}\right]^{-\frac{1}{2}}$$
$$\equiv 2^{-\frac{1}{2}}A^{-1}F(\sigma')^{-\frac{1}{2}}. \tag{22a}$$

With the use of (22), lengthy calculation gives

$$\begin{aligned}E_1=\Bigg\{&\frac{3}{2}\frac{\hbar^2}{Ma^2}\left[\left(\frac{\sigma'}{\sigma'+4}\right)^{\frac{3}{2}}\right.\\ &\left.-\frac{\sigma'^4(\sigma'+4)}{(\sigma'+1)^{5/2}(\sigma'+3)^{\frac{5}{2}}}\right](\sigma'+2)\\ &+3(1-g)\left(\frac{\sigma'^2}{\sigma'^2+6\sigma'+6}\right)^{\frac{3}{2}}A-(2-\tfrac{3}{2}g)\\ &\times\left(\frac{\sigma'}{\sigma'+3}\right)^{3}A-(1-\tfrac{3}{2}g)\left(\frac{\sigma'}{\sigma'+6}\right)^{\frac{3}{2}}A\Bigg\}\Big/F(\sigma'),\end{aligned}$$

$$s=(\tfrac{3}{2})^{\frac{1}{2}}Ag\left(\frac{\sigma}{\bar{\sigma}}\cdot\frac{\sigma'}{\bar{\sigma}}\right)^{9/4}F(\bar{\sigma})/F^{\frac{1}{2}}(\sigma'),$$

where $\bar{\sigma}=\frac{1}{2}(\sigma+\sigma')$ and F is defined by 22a.

E_1 is in the range considered very nearly a linear function of σ', rising from 10.8 Mev at $\sigma'=0$ to 65.6 Mev at $\sigma'=2$. The best value of E_0-E comes at $\sigma'\approx 1.10$, where $E_1\doteq 42$ Mev and $s\doteq 1.85$; it is 0.070 Mev, an amount which is rather insignificant in view of the inadequacies of most variation methods.

According to (19), $(b/a)^2=[(E_0-E)/s]^2$. This, with our values, is 1.4×10^{-3}. It represents the probability that in the normal state of H^3 the neutron spins shall be parallel.

III. Variation Method Applied to He^4

An application of the method described in II A to the alpha-particle entails considerable labor and has not been carried out at present. It has seemed preferable first to employ the Hartree method with the same class of functions as that used in Section II B. We know that, for H^3, this procedure misses 1/3 Mev of what the use of relative coordinates would yield, and the latter is probably in error by +1/2 Mev. The true convergence limit for He^4 is therefore expected to be probably about 1 Mev below the value obtained with the use of the present scheme.[17]

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[17] The value of σ for He^4 is 2.6 as against 1.83 for H^3. This means that the wave function is more strongly concentrated about the origin and that the *wrong* asymptotic behavior of the Hermite functions is less serious. Hence the convergence is more rapid for He^4 than for H^3 (and for H^3 than for H^2). On the other hand, the absolute error in He^4, for equal rates of convergence, is greater than for H^3 because of the greater number of $E_{\text{pot}}-E_{\text{kin}}$ terms in the Hamiltonian.

The Hamiltonian operator (11) has the form

$$H=(\hbar^2/M)\Big(-\tfrac{3}{8}\sum_i\nabla_i^2+\tfrac{1}{4}\sum_{i>j}\nabla_i\cdot\nabla_j\Big)-B\sum\nolimits_1 \times\exp[-r_{ij}^2/a^2]P_{ij}-C\sum\nolimits_2\exp[-r_{ij}^2/a^2]P_{ij}.$$

If we choose 1,2 and 3,4 to be the pairs of like particles, H is invariant with respect to the following group of permutations:

$$\begin{aligned}
P_0&=E, & P_4&=P_{13}P_{24},\\
P_1&=P_{12}, & P_5&=P_{13}P_{24}P_{12},\\
P_2&=P_{34}, & P_6&=P_{13}P_{24}P_{34},\\
P_3&=P_{12}P_{34}, & P_7&=P_{13}P_{24}P_{12}P_{34}.
\end{aligned}$$

We choose functions of the same symmetry. If this is done explicitly with the use of the P symbols in the above table, the calculation of the matrix elements is greatly facilitated. We have used the following functions

$$\phi_{000}(1)\phi_{000}(2)\phi_{000}(3)\phi_{000}(4)\qquad=\psi_0$$
$$\tfrac{1}{2}(P_0+P_1+P_4+P_7)\phi_{200}\phi_{000}\phi_{000}\phi_{000}$$
$$(1/2)^{\frac{1}{2}}(P_0+P_4)\phi_{100}\phi_{100}\phi_{000}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_2+P_3)\phi_{100}\phi_{000}\phi_{100}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_4+P_7)\phi_{400}\phi_{000}\phi_{000}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_4+P_7)\phi_{220}\phi_{000}\phi_{000}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_4+P_7)\phi_{300}\phi_{100}\phi_{000}\phi_{000}$$
$$(1/8)^{\frac{1}{2}}\sum_{i=0}^{7}P_i\phi_{300}\phi_{000}\phi_{100}\phi_{000}$$
$$(1/2)^{\frac{1}{2}}(P_0+P_4)\phi_{200}\phi_{200}\phi_{000}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_2+P_3)\phi_{200}\phi_{000}\phi_{200}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_4+P_7)\phi_{210}\phi_{100}\phi_{000}\phi_{000}$$
$$(1/8)^{\frac{1}{2}}\sum_{i=0}^{7}P_i\phi_{210}\phi_{000}\phi_{100}\phi_{000}$$
$$(1/2)^{\frac{1}{2}}(P_0+P_4)\phi_{110}\phi_{110}\phi_{000}\phi_{000}$$
$$\tfrac{1}{2}(P_0+P_1+P_2+P_3)\phi_{110}\phi_{000}\phi_{110}\phi_{000}.$$

Except in ψ_0, the arguments of the functions have not been indicated explicitly; they are understood to run consecutively. In computing the H_{ij} we make use of the invariance of H with respect to all P_i's, and look up products of the P_i in a suitably constructed group table. This allows identical terms in every H_{ij} to be recognized at once and aids in collecting them.

The potential energy terms corresponding to the previous S_{ij}, T_{ij}, U_{ij} are again separable into products of f integrals which were listed in Table II. H_{00} has its minimum value of -25.63 Mev for $\sigma=2.60$. The Coulomb energy raises this to -24.81 Mev. (This result is very sensitive to the choice of force parameters, and since these were chosen somewhat arbitrarily in this work, we do not wish to emphasize it too strongly.) The functions included in the list above contribute -1.04 Mev. This amount agrees almost exactly with that obtained by Inglis if only the second order perturbation, with a similar set of functions, is employed. The third order raises this value again by 0.25 Mev, so that the variation method, for the case of He, is more effective than perturbation theory by this amount.

We hope to return to the He^4 problem and to treat it in a manner similar to that of Section II A. For the present it seems well to be cautious in estimating the convergence limit. We feel, for reasons already mentioned, that the binding energy may lie as much as 1 Mev below the limit we have obtained. This estimate would place it at 27 Mev, not far from the experimental value, 27.6 Mev.