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Variational Theory of the Alpha-Particle

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The energy of the normal state of the alpha-particle is calculated with the use of an elaborate variational method, in which a fixed set of nuclear constants in the general symmetric Hamiltonian has been adopted. The result agrees well with an earlier, independent calculation, and allows the convergence limit to be determined with considerable precision. Comparison with previous work on H^3 indicates that the binding energies of both H^3 and He^4 can be very nearly accounted for with the use of a single set of constants satisfying the conditions imposed by the triplet state of H^2; but the value of g (ratio of Heisenberg to Majorana forces) required is lower than usually supposed, and will give somewhat too low an energy for the singlet state of H^2. The same methods are employed to calculate the excited singlet and triplet states of the alpha-particle, and yield the results which have already been stated. No excited state is stable. A virtual excited state is shown to exist near the energy of dissociation into four particles.

ALL attempts at gaining detailed knowledge of nuclear forces rely heavily upon the binding energies of light nuclei. These are known from experiments with considerable accuracy, but the theoretical methods which link them to the postulated laws of nuclear force are very uncertain indeed. Endeavors of refining these methods are therefore desirable.

Unfortunately, the nuclear four-body problem can only be solved by successive approximations. Of the method used it must be required that the energy calculated by it should converge to the true value, and preferably converge rapidly. Two general techniques are available: Schrödinger perturbation theory[1] and the variational method. As to perturbation theory it is well known that, within a given order, it does not converge to the correct energy, although the odd orders do furnish upper bounds. Hence a safe perturbational procedure must at least include the third order—the first-order result is in general poor. But the third-order perturbation is almost as difficult to calculate as the variational energy which always respresents an upper limit. Hence the variational method is employed for the most part in this paper, although occasional comparison with perturbational results is made.

The method of linear variation functions converges if the functions form a complete set, it converges rapidly if that set is chosen judiciously. But the selection of function sets is strongly limited by the practical demand of tractability. This dictates in effect that all functions shall be products of exponentially decreasing functions and polynomials. Despite this severe limitation there is some latitude inasmuch as the kind of coordinates to be adopted is not prescribed. The choice of polynomials does not affect the convergence;[2] in this work the Hermite type of polynomial is used.

Hermite functions of particle coordinates measured from a fixed fictitious center have an analytic behavior quite different from the same functions with relative coordinates as arguments. This permits two independent calculations to be made with variation functions which superficially appear identical. The use of relative and center of mass coordinates is more adapted to the nature of the problem, since it conforms in a simple way to the existence of nuclear particle groups.[3] For this reason one would expect a variation calculation in these coordinates to converge more rapidly than the other scheme which is essentially an extended Hartree method. Another advantage of the method of relative coordinates is seen in the fact that it necessitates no correction of the kinetic energy which is automatically referred to the center of mass. The price paid for these advantages is the greater labor which the method entails.

For H^3 both calculations have been made,[4] and the result is the expected one. The "Hartree method" gave an energy of -6.84 Mev with the

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[1] E. Feenberg and S. S. Share, Phys. Rev. **50**, 253 (1936); D. R. Inglis, Phys. Rev. **51**, 531 (1937).

[2] The whole calculation could be carried through with equal facility and identical results if spherical harmonics with the same radial exponential function were chosen.

[3] J. A. Wheeler, Phys. Rev. **52**, 1083 (1937).

[4] H. Margenau and D. T. Warren, Phys. Rev. **52**, 790 (1937).

use of 21 functions, the relative coordinate method yielded -7.21 Mev with only 13 functions; the same nuclear parameters were employed in both computations. In the same paper, the ground state of the alpha-particle was treated, but only in individual particle coordinates. The first part of this communication deals with the same problem and yields results which are in a sense complementary to those previously published. Besides confirming them it shows again the superiority of the relative coordinate method which, with the use of 11 functions, yields an answer better than that of the other method involving 14 rather more complicated functions. In view of this double evidence we may now estimate the true energy of the He^4 problem, and also that of H^3, more accurately than has been done before, and more definite conclusions can be drawn regarding the consistency of present assumptions about nuclear force constants.

It is generally hoped that, aside from relativity effects,[5] the binding energies of all nuclei can be fitted by a single set of nuclear force parameters. There even appears to be considerable evidence that this can be achieved by employing a Hamiltonian operator which is symmetrical in all particles[6] except for Coulomb forces. This prevailing optimism has been disturbed somewhat by the results of variational calculations on H^3 and He^4, made by Rarita and Present.[7] The present work shows, as did the former paper,[4] that a discrepancy exists, but it is not as alarming as appeared from Rarita and Present's work.

The later sections of this paper are devoted to the excited states of the alpha-particle.[8] Several estimates of the energies of these states have been made,[9] all of a very approximative character. Whereas other authors were led to believe that the P states were probably stable, our calculations, made with a more recent Hamiltonian, decide fairly definitely against their stability. Considerable effort has been made to locate the excited S state of the alpha-particle; it is found to be virtual and to lie at about 1.3 Mev above the dissociation limit.

Throughout the present work the assumption of perfect symmetry of nuclear forces, without distinction between neutrons and protons, has been made.

THE GROUND STATE

In central, individual particle coordinates, the potential interaction for all pairs of particles may be written in the general form:

$$V_{ij}=-AJ_{ij}(w+mP_{ij}+bQ_{ij}+hP_{ij}Q_{ij}), \quad (1)$$

where P_{ij} acts on coordinates, Q_{ij} on spins, and w, m, b, and h are the relative strengths of Wigner, Majorana, Bartlett, and Heisenberg forces, respectively. If the coordinate part of the variation functions is chosen symmetric in like particles, a summation over spins leads to an interaction:[10]

$$\begin{aligned}(V_{ij})_1&=-AJ_{ij}[(w+\tfrac{1}{2}b)+(m+\tfrac{1}{2}h)P_{ij}],\\(V_{ij})_2&=-AJ_{ij}[(w-b)+(m-h)P_{ij}],\end{aligned} \quad (2)$$

where the subscripts 1 and 2 refer to interactions between pairs of unlike and like particles, respectively.

As in the previous work,[4] the Gaussian form of interaction is used; thus $J_{ij}=\exp(-r_{ij}^2/a^2)$.

It has been pointed out by Breit and Feenberg[11] that the effect of the P_{ij} operators is very small inasmuch as the ground state of the alpha-particle is nearly symmetric in all particles. This will be discussed in more detail later. In the above expressions, the Majorana coefficient is predominant. Therefore it will be a good

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[5] G. Breit, Phys. Rev. **53**, 153 (1938).

[6] M. A. Tuve, N. P. Heydenburg and L. R. Hafstad, Phys. Rev. **50**, 806 (1936); G. Breit, E. U. Condon, R. D. Present, Phys. Rev. **50**, 825 (1936); E. Wigner, Phys. Rev. **51**, 106 (1936).

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

[8] When this manuscript was completed there appeared a paper by S. S. Share, Phys. Rev. **53**, 875 (1938), which contains some of the results here obtained. Since our method of attack is different, a more general Hamiltonian has been used, and the excited S state has been investigated in greater detail, we are persuaded not to withdraw these sections from publication. Share's result on the excited S state of He^4 is not significant because his energy does not represent an upper limit. Our result does represent such a limit.

[9] E. Feenberg, Phys. Rev. **49**, 328 (1936); Bethe and Bacher, Rev. Mod. Phys. **8**, 82 (1936).

[10] This is obvious for like particles; for unlike particles, cf. Bethe and Bacher, Rev. Mod. Phys. **8**, 82 (1936).

[11] G. Breit and E. Feenberg, Phys. Rev. **50**, 850 (1936).

approximation to write

$$(V_{ij})_1 = -AJ_{ij}[w+m+\tfrac{1}{2}(b+h)]P_{ij} = -BJ_{ij}P_{ij},$$
$$(V_{ij})_2 = -AJ_{ij}[w+m-(b+h)]P_{ij} = -CJ_{ij}P_{ij}. \tag{3}$$

If now $b+h=g$, then $B=(1-\frac{1}{2}g)A$, $C=(1-2g)A$.

The Coulomb energy, small compared with the total energy, will be omitted from the variational calculation and taken into account afterwards. Hence the Hamiltonian in central, individual particle coordinates is

$$H = -(\hbar^2/2M)\sum_i \nabla_i^2 - B\sum_{ij}{}_1 J_{ij}P_{ij} - C\sum_{ij}{}_2 J_{ij}P_{ij}, \tag{4}$$

where $\sum_1$ is extended over pairs of unlike, and $\sum_2$ over pairs of like particles. This is the same Hamiltonian which was employed for H^3 (cf. Eq. (2), reference 4).

In order to facilitate comparison of the present work with the results for H^3, the following values of the constants have been assumed:

$$A = 35.60 \text{ Mev}, \quad a = 2.25\times 10^{-13} \text{ cm}, \quad g = 0.194$$

which give

$$B = 32.10 \text{ Mev}, \quad C = 21.77 \text{ Mev}.$$

The transformation to relative coordinates is:

$$\boldsymbol{\varrho}_1 = (\tfrac{1}{2})^{\frac{1}{2}}(\mathbf{r}_1+\mathbf{r}_2-\mathbf{r}_3-\mathbf{r}_4);$$
$$\boldsymbol{\varrho}_2 = (\tfrac{1}{2})^{\frac{1}{2}}(\mathbf{r}_1-\mathbf{r}_2); \quad \boldsymbol{\varrho}_3 = (\tfrac{1}{2})^{\frac{1}{2}}(\mathbf{r}_3-\mathbf{r}_4). \tag{5}$$

Since this transformation, the interaction J_{ij}, and, as will be seen below, the form of variation function are all symmetric with respect to the Cartesian axes, attention may be confined to the scalar X component equations in much of what follows. Taking ξ_i, η_i, ζ_i to be the rectangular components of the relative vectors $\boldsymbol{\varrho}_i$, we find:

$$x_{12} = 2^{\frac{1}{2}}\xi_2; \qquad x_{13} = (\tfrac{1}{2})^{\frac{1}{2}}(\xi_1+\xi_2-\xi_3)$$
$$x_{14} = (\tfrac{1}{2})^{\frac{1}{2}}(\xi_1+\xi_2+\xi_3); \quad x_{23} = (\tfrac{1}{2})^{\frac{1}{2}}(\xi_1-\xi_2-\xi_3)$$
$$x_{24} = (\tfrac{1}{2})^{\frac{1}{2}}(\xi_1-\xi_2+\xi_3); \quad x_{34} = 2^{\frac{1}{2}}\xi_3.$$

This leads to Table I, which gives the effect of the permutation operators P_{ij} upon the ξ_i.

The Hamiltonian may now be written in relative coordinates. Eq. (4) becomes

$$\begin{aligned} H = &-(\hbar^2/2M)(2\nabla_1^2+\nabla_2^2+\nabla_3^2) \\ &-B\{\exp[-\tfrac{1}{2}\tau(\boldsymbol{\varrho}_1+\boldsymbol{\varrho}_2-\boldsymbol{\varrho}_3)^2]P_{13} \\ &+\exp[-\tfrac{1}{2}\tau(\boldsymbol{\varrho}_1+\boldsymbol{\varrho}_2+\boldsymbol{\varrho}_3)^2]P_{14} \\ &+\exp[-\tfrac{1}{2}\tau(\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_2-\boldsymbol{\varrho}_3)^2]P_{23} \\ &+\exp[-\tfrac{1}{2}\tau(\boldsymbol{\varrho}_1-\boldsymbol{\varrho}_2+\boldsymbol{\varrho}_3)^2]P_{24}\} \\ &-C\{\exp[-2\tau\boldsymbol{\varrho}_2^2]P_{12} \\ &\qquad +\exp[-2\tau\boldsymbol{\varrho}_3^2]P_{34}\}, \end{aligned} \tag{6}$$

where $\tau = 1/a^2$. Eq. (6) is symmetric with respect to an interchange of coordinates 2 and 3. This necessitates the use of variation functions symmetric in coordinates 2 and 3, because the ground state of He^4 is nondegenerate and hence possesses the same symmetry as the Hamiltonian. Furthermore, an interchange of the protons (particles 1 and 2), or of the neutrons causes a change of sign in $\boldsymbol{\varrho}_2$ or $\boldsymbol{\varrho}_3$, respectively. Therefore, all variation functions must be even functions of relative coordinates 2 and 3, in order that they may be symmetric coordinate functions.

As in the work on H^3, single harmonic oscillator functions are employed for variation functions. The notation for these functions is as follows: Single Hermite functions are written

$$\varphi_n(p^{\frac{1}{2}}x) = \varphi_n{}^p(x) = N_{n,\,p}\exp(-px^2/2)H_n(p^{\frac{1}{2}}x),$$

where $N_{n,\,p}$ is a normalizing factor, H_n is a Hermite polynomial, and x may be any of the rectangular components of $\boldsymbol{\varrho}_1$, $\boldsymbol{\varrho}_2$, $\boldsymbol{\varrho}_3$. Then we define

$$\varphi_{lmn}(i) = \varphi_l(\xi_i)\varphi_m(\eta_i)\varphi_n(\zeta_i),$$

and these functions can be symmetrized with respect to the Cartesian axes by forming

$$\begin{aligned} \phi_{lmn} = &(\tfrac{1}{6})^{\frac{1}{2}}(1+\delta_{lm}+\delta_{ln}+\delta_{mn}+2\delta_{lm}\delta_{ln}\delta_{mn})^{-\frac{1}{2}} \\ &\times(\varphi_{lmn}+\varphi_{lnm}+\varphi_{nlm}+\varphi_{mln}+\varphi_{mnl}+\varphi_{nml}). \end{aligned} \tag{7}$$

TABLE I. *The effect of the P_{ij} operators upon the ξ_i.*

P_{ij}	$P_{ij}\xi_1$	$P_{ij}\xi_2$	$P_{ij}\xi_3$
P_{12}	ξ_1	$-\xi_2$	ξ_3
P_{13}	$-\xi_2+\xi_3$	$\frac{1}{2}(-\xi_1+\xi_2+\xi_3)$	$\frac{1}{2}(\xi_1+\xi_2+\xi_3)$
P_{14}	$-\xi_2-\xi_3$	$\frac{1}{2}(-\xi_1+\xi_2-\xi_3)$	$\frac{1}{2}(-\xi_1-\xi_2+\xi_3)$
P_{23}	$\xi_2+\xi_3$	$\frac{1}{2}(\xi_1+\xi_2-\xi_3)$	$\frac{1}{2}(\xi_1-\xi_2+\xi_3)$
P_{24}	$\xi_2-\xi_3$	$\frac{1}{2}(\xi_1+\xi_2+\xi_3)$	$\frac{1}{2}(-\xi_1+\xi_2+\xi_3)$
P_{34}	ξ_1	ξ_2	$-\xi_3$

The variation parameters p determine the classical potentials for the oscillator functions; since all variation functions are chosen symmetric in coordinates 2 and 3, two, rather than three such parameters are needed. In the work that follows, it will be implicit that p is the parameter for coordinate 1 and q for coordinates 2 and 3. To give an explicit example of the notation employed,

$$\phi_{200}(1)\phi_{000}(2)\phi_{000}(3)=(\tfrac{1}{3})^{\frac{1}{2}}[\varphi_2{}^p(\xi_1)\varphi_0{}^p(\eta_1)\varphi_0{}^p(\zeta_1)$$
$$+\varphi_0{}^p(\xi_1)\varphi_2{}^p(\eta_1)\varphi_0{}^p(\zeta_1)+\varphi_0{}^p(\xi_1)\varphi_0{}^p(\eta_1)\varphi_2{}^p(\zeta_1)]$$
$$\times\varphi_0{}^q(\xi_2)\varphi_0{}^q(\eta_2)\varphi_0{}^q(\zeta_2)\times\varphi_0{}^q(\xi_3)\varphi_0{}^q(\eta_3)\varphi_0{}^q(\zeta_3).$$

The single function which gives the lowest energy is $\psi_0=\phi_{000}(1)\phi_{000}(2)\phi_{000}(3)$, hereinafter designated as the ground state function. No functions have been used variationally which do not combine with the ground state function. This eliminates all functions of odd degree of excitation, and, in addition, certain functions of even degree. As can be readily shown from the nature of the integrals below, in general those functions which do not combine with ψ_0 have also vanishing matrix elements with functions combining with ψ_0. It is thus clear that functions which do not combine with the ground state are unimportant variationally.

A list of all functions of low excitation which combine with ψ_0 follows:

Ground state function:

$$\psi_0=\phi_{000}(1)\phi_{000}(2)\phi_{000}(3)$$

Doubly excited:

$\phi_{200}(1)\phi_{000}(2)\phi_{000}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{200}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{200}(3)].$

Quadruply excited:

$\phi_{400}(1)\phi_{000}(2)\phi_{000}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{400}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{400}(3)].$
$\phi_{000}(1)\phi_{200}(2)\phi_{200}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{200}(1)[\phi_{200}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{200}(3)]$
$\phi_{000}(1)\phi_{110}(2)\phi_{110}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{110}(1)[\phi_{110}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{110}(3)]$
$\phi_{220}(1)\phi_{000}(2)\phi_{000}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{220}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{220}(3)].$

Sextuply excited:

$\phi_{200}(1)\phi_{200}(2)\phi_{200}(3)$
$\phi_{600}(1)\phi_{000}(2)\phi_{000}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{600}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{600}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{400}(1)[\phi_{200}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{200}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{200}(1)[\phi_{400}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{400}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{400}(2)\phi_{200}(3)+\phi_{200}(2)\phi_{400}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{220}(1)[\phi_{200}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{200}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{200}(1)[\phi_{220}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{220}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{220}(2)\phi_{200}(3)+\phi_{200}(2)\phi_{220}(3)]$
$\phi_{200}(1)\phi_{110}(2)\phi_{110}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{110}(1)[\phi_{200}(2)\phi_{110}(3)+\phi_{110}(2)\phi_{200}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{310}(1)[\phi_{110}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{110}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{110}(1)[\phi_{310}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{310}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{310}(2)\phi_{110}(3)+\phi_{110}(2)\phi_{310}(3)]$
$\phi_{222}(1)\phi_{000}(2)\phi_{000}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{222}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{222}(3)]$
$\phi_{420}(1)\phi_{000}(2)\phi_{000}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{420}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{420}(3)]$
$\phi_{110}(1)\phi_{110}(2)\phi_{110}(3)$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{211}(1)[\phi_{110}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{110}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{110}(1)[\phi_{211}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{211}(3)]$
$(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{211}(2)\phi_{110}(3)+\phi_{110}(2)\phi_{211}(3)].$

There are 61 octuply excited functions which could be added to the list. The importance of these and higher excited functions will be discussed later.

The evaluation of the matrix element $H_{ij}=\int\psi_iH\psi_jd\tau$ divides into three parts: the evaluation of the kinetic energy, the unlike particle interaction, and the like particle interaction.

To find the kinetic energy, it is to be noted that the function

$$\psi=\varphi n_{\xi_1}(p^{\frac{1}{2}}\xi_1)\varphi n_{\eta_1}(p^{\frac{1}{2}}\eta_1)\varphi n_{\zeta_1}(p^{\frac{1}{2}}\zeta_1)$$
$$\times\varphi n_{\xi_2}(q^{\frac{1}{2}}\xi_2)\cdots\varphi n_{\zeta_3}(q^{\frac{1}{2}}\zeta_3)$$

satisfies the equation

$$(\hbar^2/2M)\{-(2\nabla_1{}^2+\nabla_2{}^2+\nabla_3{}^2)$$
$$+[2p^2\rho_1{}^2+q^2(\rho_2{}^2+\rho_3{}^2)]\}\psi=E\psi,$$

and the eigenvalues are

$$E(n_{\xi_1}\cdots n_{\zeta_3})=(\hbar^2/M)\Big[\Big(\sum_{\xi\eta\zeta}n_1+\tfrac{3}{2}\Big)2p$$
$$+\Big\{\sum_{\xi\eta\zeta}(n_2+n_3)+3\Big\}q\Big]. \quad (8)$$

Hence

$$(E_{\mathrm{kin}})_{ij}=\int\psi_i[-(\hbar^2/2M)(2\nabla_1^2+\nabla_2^2+\nabla_3^2)]\psi_j d\tau$$
$$=E\delta_{ij}-(\hbar^2/2M)\int\psi_i[2p^2\rho_1^2$$
$$+q^2(\rho_2^2+\rho_3^2)]\psi_j d\tau, \quad (9)$$

since the functions are orthogonal and normalized. Moreover, the last part of Eq. (9),

$$2p\int\psi_i p\rho_1^2\psi_j d\tau+q\int\psi_i q\rho_2^2\psi_j d\tau+q\int\psi_i q\rho_3^2\psi_j d\tau,$$

breaks up into integrals of the form

$$\int\varphi_i^p(\xi)p\xi^2\varphi_j^p(\xi)d\xi\equiv\lambda_{ij}=(i+\tfrac{1}{2})\delta_{ij}$$
$$+\tfrac{1}{2}[(i+1)(i+2)]^{\frac{1}{2}}\delta_{j,\,i+2},$$

so that the matrix elements of the kinetic energy can be written as sums of various λ_{ij}.

If we set

$$R_{ij}\equiv\int\psi_i\exp[-\tfrac{1}{2}\tau(\varrho_1+\varrho_2+\varrho_3)^2]P_{14}\psi_j d\tau,$$

$$S_{ij}\equiv\int\psi_i\exp[-\tfrac{1}{2}\tau(\varrho_1+\varrho_2-\varrho_3)^2]P_{13}\psi_j d\tau,$$

$$T_{ij}\equiv\int\psi_i\exp[-\tfrac{1}{2}\tau(\varrho_1-\varrho_2-\varrho_3)^2]P_{23}\psi_j d\tau,$$

$$U_{ij}\equiv\int\psi_i\exp[-\tfrac{1}{2}\tau(\varrho_1-\varrho_2+\varrho_3)^2]P_{24}\psi_j d\tau,$$

then the unlike particle interaction part of H_{ij} is

$$-B(R_{ij}+S_{ij}+T_{ij}+U_{ij}).$$

R_{ij} may be written as the product of three integrals, one for each rectangular component. Replacing $(\psi_i)_x$ and $(\psi_j)_x$ by ϕ_{lmn} functions, we see that the basic integral is

$$r_{ijk,\,lmn}=\int\varphi_i^p(\xi_1)\varphi_j^q(\xi_2)\varphi_k^q(\xi_3)$$
$$\times\exp[-\tfrac{1}{2}\tau(\xi_1+\xi_2+\xi_3)^2]P_{14}\varphi_l^p(\xi_1)$$
$$\times\varphi_m^q(\xi_2)\varphi_n^q(\xi_3)d\xi_1 d\xi_2 d\xi_3$$

and that then R_{ij} is expressible as a sum of products of three $r_{ijk,\,lmn}$. To facilitate integration, a transformation

$$\xi_1=s;\quad \xi_2=\tfrac{1}{2}(u+t);\quad \xi_3=\tfrac{1}{2}(u-t) \quad (10)$$

is made; Table II gives the effect of the P_{ij} operators upon ξ_i in terms of u, s, t.

The effect of the P_{ij} operators upon $\varphi_l\varphi_m\varphi_n$ can be expressed by their effect upon the arguments of these functions; hence

$$r_{ijk,\,lmn}=\int\varphi_i^p(s)\varphi_j^q\Big(\frac{u+t}{2}\Big)\varphi_k^q\Big(\frac{u-t}{2}\Big)$$
$$\times\exp(-\tfrac{1}{2}\tau(s+u)^2)\varphi_l^p(-u)$$
$$\times\varphi_m^q\Big(\frac{t-s}{2}\Big)\varphi_n^q\Big(\frac{-t-s}{2}\Big)dsdtdu,$$
$$=\tfrac{1}{2}\int H_i(p^{\frac{1}{2}}s)\cdots H_l(-p^{\frac{1}{2}}u)\cdots Idsdtdu,$$

where

$$I\equiv\varphi_0^p(s)\varphi_0^q\Big(\frac{u+t}{2}\Big)\varphi_0^q\Big(\frac{u-t}{2}\Big)\varphi_0^p(-u)$$
$$\times\varphi_0^q\Big(\frac{t-s}{2}\Big)\varphi_0^q\Big(\frac{-t-s}{2}\Big)\exp(-\tfrac{1}{2}\tau(s+u)^2),$$

and $\frac{1}{2}$ is the Jacobian of the transformation. From the form of I, it may be seen that $r_{ijk,\,lmn}$ vanishes unless $i+j+k$ is of the same parity as $l+m+n$.

A similar procedure is carried through for S_{ij}, T_{ij}, U_{ij}, which gives basic integrals $s_{ijk,\,lmn}$, $t_{ijk,\,lmn}$, $u_{ijk,\,lmn}$, respectively, which the reader can easily construct with the aid of Table II.

In the integrand of $s_{ijk,\,lmn}$, u and t may be interchanged. This makes $s_{ijk,\,lmn}$ identical with $r_{ijk,\,lmn}$, except that the arguments of φ_k and φ_n are reversed in sign. Hence

$$s_{ijk,\,lmn}=(-1)^{k+n}r_{ijk,\,lmn}. \quad (11a)$$

TABLE II. *The effect of P_{ij} upon ξ_i in terms of u, s, t.*

P_{ij}	$P_{ij}\xi_1$	$P_{ij}\xi_2$	$P_{ij}\xi_3$
P_{12}	s	$-\frac{1}{2}(u+t)$	$\frac{1}{2}(u-t)$
P_{13}	$-t$	$\frac{1}{2}(-s+u)$	$\frac{1}{2}(s+u)$
P_{14}	$-u$	$\frac{1}{2}(-s+t)$	$-\frac{1}{2}(s+t)$
P_{23}	u	$\frac{1}{2}(s+t)$	$\frac{1}{2}(s-t)$
P_{24}	t	$\frac{1}{2}(s+u)$	$\frac{1}{2}(-s+u)$
P_{34}	s	$\frac{1}{2}(u+t)$	$\frac{1}{2}(t-u)$

In the integrand of $t_{ijk,\ lmn}$, a change of the signs of t and u throughout yields

$$t_{ijk,\ lmn}=(-1)^{j+k+m+n}r_{ijk,\ lmn}, \tag{11b}$$

and by similar reasoning we find

$$u_{ijk,\ lmn}=(-1)^{j+m}r_{ijk,\ lmn}. \tag{11c}$$

It will be noted that

$$-B(R_{ij}+S_{ij}+T_{ij}+U_{ij})=-4BR_{ij} \text{ or } 0, \tag{11d}$$

depending upon the values of j, k, m, n in the basic integrals encountered. These rules make it easy to pick out functions which combine with each other. Lists of over 100 of the various $r_{ijk,\ lmn}$ have been prepared, but will not be reproduced here.

If we put

$$V_{ij}\equiv\int\psi_i \exp\left[-2\tau\rho_2{}^2\right]P_{12}\psi_j d\tau$$

$$W_{ij}\equiv\int\psi_i \exp\left[-2\tau\rho_3{}^2\right]P_{34}\psi_j d\tau,$$

then the like particle interaction part of H_{ij} is

$$-C(V_{ij}+W_{ij}).$$

V_{ij} is the product of three integrals, one for each rectangular axis; and it is necessary to consider only one of them. P_{12} leaves ξ_1 and ξ_3 unchanged (cf. Table I); integration over ξ_1 and ξ_3 yields unity. Now let

$$v_{ij}\equiv\int\varphi_i{}^q(\xi_2)\exp\left[-2\tau\xi_2{}^2\right]P_{12}\varphi_j{}^q(\xi_2)d\xi_2$$

$$=\int H_i(q^{\frac{1}{2}}\xi_2)H_j(-q^{\frac{1}{2}}\xi_2)$$

$$\times\left[\varphi_0{}^q(\xi_2)\varphi_0{}^q(-\xi_2)\exp\left(-2\tau\xi_2{}^2\right)\right]d\xi_2.$$

Then V_{ij} will be expressible as a sum of products of three v_{ij}. From the form of the bracketed expression, it may be proved that v_{ij} vanishes unless i is of the same parity as j. Only eight different v_{ij} appear in V_{ij} for all the doubly and quadruply excited variation functions listed above.

Furthermore, $W_{ij}=V_{ij}$ because all functions ψ_i are symmetric in relative coordinates 2 and 3.

When Wigner forces are introduced, integrals of the types above without exchange operators are needed. These can of course be calculated in a similar manner, or more directly without the use of the transformation (10). In the following, integrals will be understood to refer to Majorana forces if no further designation is given. When the necessity for distinction arises, integrals involving Wigner and Majorana forces will be labeled by superscripts W and M, respectively. It is to be noted here that the relations (11) hold for Wigner terms also.

In order to obtain the variational energy, we must solve for the lowest root E_1 of the determinantal equation $|H_{ij}-\delta_{ij}E|=0$. It is obviously too laborious to retain p and q as variation parameters throughout the solution. However, the minimum of H_{00} occurs at $2p=q=0.5135$, and H_{00} accounts for most of the binding energy. Therefore the values of p and q which minimize E_1 will not differ appreciably from these values, and it is safe to evaluate H_{ij} at the minimum of H_{00}, before insertion in the determinant. This procedure has been followed here; the numerical method of solving the secular equation has been outlined elsewhere.[4]

Since the numerical values of H_{0i} are available from the variational calculation, it is very simple also to make a second order Schrödinger perturbation calculation by use of the same functions. In this scheme, the additional energy is

$$E^{(2)}=\sum_i{}'\frac{H_{0i}{}^2}{E_0-E_i}$$

and it is clear from Eq. (8) that

$$E_0-E_i=-\frac{\hbar^2}{M}\sum\left\{(n_i)_\xi+(n_i)_\eta+(n_i)_\zeta\right\}q,$$

if $q=2p$. Thus the denominator will be the same for all functions of the same degree of excitation.

TABLE III. *Results of variational and perturbational calculations for the ground state of* He^4 (*in Mev*).

No. of Functions	E_1	E_1-H_{00}	$E^{(2)}$	$\frac{E_1-H_{00}}{E^{(2)}}$
4	-26.29	-0.60	-0.50	1.20
5	-26.41	-0.72	-0.59	1.22
8	-26.52	-0.83	-0.74	1.12
11	-26.76	-1.07	-0.81	1.32
33			-0.93	

Table III lists the results of the variational and perturbational calculations. The most elaborate variational calculation has been made with the ground state function and all the doubly and quadruply excited functions, a total of 11 variation functions. The result is in excellent agreement with a former calculation[4] by an entirely independent scheme (individual particles coordinates) which gave -26.67 Mev.

It will be seen that the variation method gives a lowering of the total energy slightly greater than that of second order perturbation theory with the same set of functions. The ratio between the contributions varies somewhat irregularly for different stages of the calculation; after inclusion of all the quadruply excited functions, it is 1.32. By adjusting the perturbational energy for all the sextuply excited functions, we feel that a close estimate of the variational energy due to these functions (in relative coordinates) may be obtained; multiplication of 0.12 by 1.32 yields 0.16 Mev for this estimate.

The division of functions into classes of various degrees of excitation is quite dependent upon the type of coordinates employed; in relative coordinates, the set of sextuply excited functions is equivalent to some of the sextuply excited, and many of the octuply excited functions in individual particle coordinates. Hence 0.16 Mev also represents a *rough* estimate of the effect of octuply excited functions in individual particle coordinates. We may at least say, then, that octuply excited states make a very small contribution to the total energy of the alpha-particle. This is not true in the deuteron problem.[12]

Perturbational results show that functions higher than octuply excited have a negligible effect upon the ground state. Thus, allowing a contribution of -0.33 Mev for the effect of sextuply and octuply excited states, we obtain -27.09 Mev as a fairly close estimate for the convergence limit of the variational energy. The Coulomb energy is $+0.82$ Mev; therefore the final figure for the energy of the ground state of He^4 is -26.27 Mev.

As already mentioned, the foregoing results involve the approximation of treating the Wigner part of (2) as though it were a Majorana operator. The effect of this approximation may be easily traced through the first-order calculation leading to H_{00}. Since it is small in H_{00}, it will be completely neglected in the higher contributions.

Let H be the operator (4), used in this work, and $\mathcal{H}$ the same operator, but without the P_{ij}'s. Then H_{00} and $\mathcal{H}_{00}$ will in general have separate minima.[13] If $B=C$, the two minima coincide and occur at $\lambda=1$. In that case no correction at all is necessary. For the values of B and C adopted in this paper, this coincidence is not quite present. But it is seen from Fig. 1, where both H_{00} and $\mathcal{H}_{00}$ are plotted as functions of λ at the minimum with respect to σ, that the correction is small indeed. To give an idea of the correction required in the worst possible case ($C=0$) we have plotted similar curves representing that situation in the lower part of Fig. 1. It is seen that even there the two minima differ by less than $\frac{1}{2}$ Mev in energy. Hence it is clear that the effect of ignoring the "ordinary" constituent of the nuclear forces is quite inappreciable in dealing with the ground state of He^4. The same is true for H^3.

It is now possible to test the adequacy of the symmetrical Hamiltonian in reference to the two important problems: H^3 and He^4. The present results and those obtained previously[4] are gained with the same nuclear constants, and by the same method. We feel that the value of the binding energy of He^4 here derived probably represents a closer estimate than that for H^3. On the other hand, further experience with the present method has led us to believe that the margin of uncertainty in its convergence for H^3

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[12] D. T. Warren and H. Margenau, Phys. Rev. **52**, 1027 (1937).

[13] Algebraic expressions for H_{00} and $\mathcal{H}_{00}$ may be found in the papers of Wigner, Phys. Rev. **43**, 252 (1933), Feenberg, Phys. Rev. **47**, 850 (1935) and others. For the definition of the variation parameters λ and σ see Eq. (13).

is far smaller than was judged by Margenau and Warren. We prefer to assume that the result for the binding energy of H^3 is 7.3 Mev (7.21 being actually obtained variationally). If it is *greater*, the discrepancy (Eqs. (12)) to which this analysis leads, will be *less* pronounced.[14]

Slight adjustments in the constants B and C will not change the contributions of the higher variation functions appreciably. We shall therefore inquire what changes in B and C are necessary so that H_{00}, computed with the adjusted values of these parameters, plus the uncorrected higher contributions, shall equal the observed binding energies for both H^3 and He^4. Table IV shows the procedure. The last row shows the energy to be accounted for by the ground state function ψ_0.* Working with the minimizing values of λ and σ we then determine B and C from the equations for H_{00}.

$$\left.\begin{array}{ll} H^3: & -7.20=22.09-0.669B-0.314C \\ He^4: & -27.0=47.37-1.70B-0.850C \end{array}\right\}.$$

They yield:

$$\begin{array}{lll} H^3: & B=32.6\text{ Mev}, & C=23.8\text{ Mev}, \\ He^4: & B=32.4\text{ Mev}, & C=22.0\text{ Mev}, \end{array}$$

which reveal a slight inconsistency. Remembering that $B=(1-\frac{1}{2}g)A$, $C=(1-2g)A$, we find

$$H^3:\ g=0.167,\quad He^4:\ g=0.181. \tag{12}$$

It is to be noted first that these values of g are considerably smaller than that usually derived from the ${}^1S-{}^3S$ energy spacing of the deuteron states.

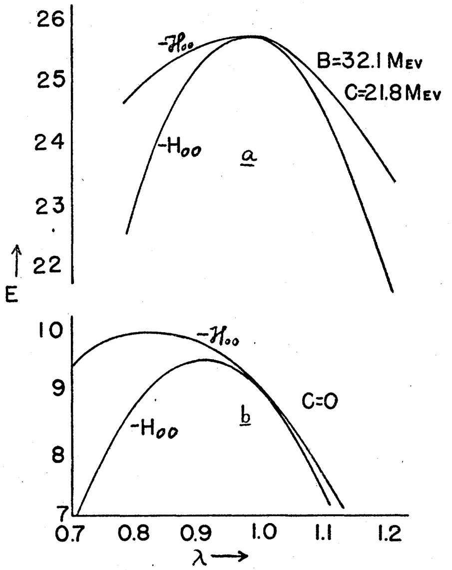

FIG. 1. Variational binding energy of He^4 in zero*th* approximation with (H_{00}) and without ($\mathcal{H}_{00}$) exchange forces: (a) $B=32.1$ Mev, $C=21.77$ Mev; (b) $B=32.1$ Mev, $C=0$.

The significance of the discrepancy inherent in (12) is best seen by computing the binding energies of H^3 and He^4 with an artificial *mean* value of g, equal to 0.174. This yields 8.1 Mev and 28.3 Mev, which differ from the experimental results by -0.2 and $+0.7$ Mev, respectively. The discrepancy has the same sense as that found by Rarita and Present, but is less severe. It is to be noted, however, that this improved agreement involves the use of a value of g which differs considerably from that of Rarita and Present (0.215), and one which leads to a stable singlet state of the deuteron. We may thus say: The strong discrepancy in the binding energy of light nuclei emphasized by Rarita and Present may be made much less pronounced by choosing a smaller value of the ratio of Heisenberg to Majorana forces. In fact, by taking g as small as 0.174 the discrepancy almost vanishes. While it is unlikely that such a value is compatible with

TABLE IV. *Computation of* H_{00}.

	H^3	He^4
Experimental energy	-8.3	-27.6
Coulomb energy	0	$+0.8$
Contributions from functions other than ψ_0	-1.1	-1.4
H_{00}	-7.2	-27.0

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[14] In his review article Breit (Rev. Sci. Inst. 9, 63 (1939)) mentions the existence of a disagreement between the results of Rarita and Present and those of Margenau and Warren. We fear that excessive caution on the part of the latter authors in estimating the convergence limit of their method is responsible for this impression. The numerical results certainly show no contradiction, for, with the adopted set of constants Margenau and Warren obtained binding energies of 7.21 for H^3 and 25.85 for He^4. If these had been taken at face value the same qualitative conclusion as that drawn by Rarita and Present would have resulted, as was stated. Whether one method converges faster than the other is at present unknown, and all estimates of convergence limits must be regarded as plausible subjective judgments. A direct quantitative comparison of the results of the two papers in question is not feasible because of the different form of the potentials adopted.

* We are neglecting (a) the effect of states in which the spins are distributed differently among the particles; (b) relativity corrections. (a) is of the same magnitude as the estimated error in the convergence limit; (b) is probably appreciable but at present impossible to calculate uniquely.

scattering data, a compromise value around 0.19 might bring the discrepancy within the range of errors caused by the neglect of relativity and other corrections.

EXCITED S STATE

We are concerned here with an excited state possessing the same symmetry as the ground state. An upper bound to the position of the state may therefore be obtained by solving $|H_{ij}-\delta_{ij}E|=0$ for E_2, the next highest root above E_1. It is not possible, however, to find any one variation function for which H_{ii} is a *good* approximation to E_2. Hence we cannot use the minimization procedure which was followed in locating E_1; instead, it is necessary to minimize E_2 directly with respect to one or both of the variation parameters.

Careful study was made with the following set of functions in relative coordinates:

$$\psi_0=\phi_{000}(1)\phi_{000}(2)\phi_{000}(3)$$

$$\psi_1=(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{200}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{200}(3)]$$

$$\psi_2=\phi_{200}(1)\phi_{000}(2)\phi_{000}(3)$$

$$\psi_3=(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{400}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{400}(3)].$$

The Hamiltonian given by Eq. (6) was used; the matrix elements may then be evaluated by the technique developed for the ground state. Instead of the variation parameters p and q, it is more convenient to write

$$p=(2-\lambda)\sigma\tau;\quad q=2\lambda\sigma\tau. \tag{13}$$

Of the ten matrix elements involving the foregoing functions, we shall give here only the three diagonal ones which seem of principal interest, and omit the others because of their length.

Let

$$\begin{aligned} r&\equiv r_{000,\,000}=\lambda^{\frac{1}{2}}(2-\lambda)^{\frac{1}{2}}\left(\frac{\sigma}{\sigma+1}\right)^{\frac{1}{2}} \\ v&\equiv v_{00}=\left(\frac{\lambda\sigma}{\lambda\sigma+1}\right)^{\frac{1}{2}}. \end{aligned} \tag{14}$$

Then:

$$H_{00}=3(2+\lambda)(4.05)\sigma-4Br^3-2Cv^3,$$

$$\begin{aligned} H_{11}=(6+7\lambda)(4.05)\sigma & \\ -4B\left[\frac{5}{4}-\frac{3}{2}\lambda\left(\frac{\sigma+\frac{1}{2}}{\sigma+1}\right)+\frac{3}{4}\lambda^2\frac{\sigma^2+\sigma+5/12}{(\sigma+1)^2}\right]r^3 & \\ -2C\left[\frac{\lambda^2\sigma^2+\lambda\sigma+5/4}{(\lambda\sigma+1)^2}\right]v^3 & \end{aligned}$$

$$\begin{aligned} H_{22}=(14-\lambda)(4.05)\sigma-4B\left[\frac{3}{2}-3(2-\lambda)\left(\frac{\sigma+\frac{1}{2}}{\sigma+1}\right)\right. & \\ \left.+\frac{3}{2}(2-\lambda)^2\frac{\sigma^2+\sigma+5/12}{(\sigma+1)^2}\right]r^3-2Cv^3, & \end{aligned}$$

where 4.05 Mev has been put for $\hbar^2\tau/2M$.

A preliminary investigation showed that ψ_1 contributes the most to the excited S state, since H_{11} lies lower than any other H_{ii} except H_{00}. In fact, it possesses a minimum, which, however, is not to be interpreted as an excited state, for H_{11} is quite different from the second root, E_2. The position of the latter results from a compromise between the tendency of ψ_0 to raise H_{11}, and that of the higher functions to depress it.

The lowest curve for H_{11} *vs.* σ is obtained by putting $\lambda=\frac{2}{3}$ (which corresponds to $p=q$). Accordingly, all matrix elements in the secular equation are evaluated at $\lambda=\frac{2}{3}$; it then becomes necessary to find E_2 as a function of σ. It is possible, of course, that E_2 has a groove for a somewhat different value of λ, but a detailed study of this matter has not seemed to us worth while.

Figure 2 shows the dependence of H_{11} and E_2 upon σ. It is seen that E_2 shows a shallow minimum at about $\sigma=0.425$, and the value of E_2 is 1.3 Mev at this minimum. We believe that the inclusion of further functions in the variational calculation would not lower this minimum appreciably; it is questionable that it would be pushed into the discrete spectrum at all.

This state is not stable against disintegration into H^3+p, or into He^3+n, or into two deuterons. If virtual, the level is not even stable against disintegration into four particles. However, $1/\sigma^{\frac{1}{2}}$ is a measure of the mean distance of separation of the particles in units a: Fig. 2 is equivalent to a plot of total energy *vs.* distance. Hence, as we bring the particles together, there is a shallow

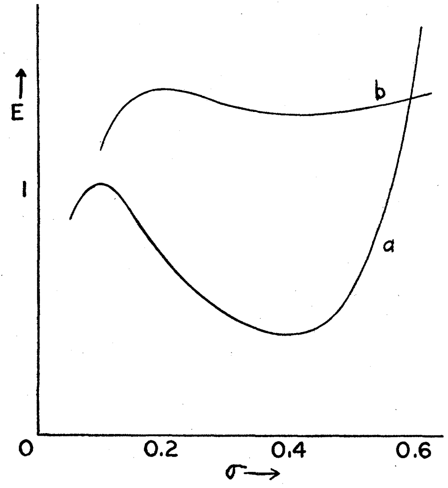

FIG. 2. Energy of excited S state in Mev for $\lambda=\frac{2}{3}$. a: H_{11}; b: Second root, E_2.

minimum in which they may vibrate. The minimizing value of σ for the ground state is 1.3; thus, for the excited S state, the mean distance of separation of the particles is about 1.75 times as great as for the ground state.

The existence of this theoretically predicted excited state is, of course, of no importance in nuclear statics; but it should give rise to a resonance peak in certain scattering and disintegration processes, as, for example, in the deuteron-deuteron reaction.

SINGLET *P* STATE

P states are odd in one coordinate and do not combine with the ground state of the alpha-particle. Therefore in determining the energy of the lowest P state, the variational method is just as easy to apply as in working for the ground state; it is merely necessary to select functions of the proper symmetry and to solve for the lowest root of the determinantal equation. It is not quite proper to use the Hamiltonian in the simple form (3). Nevertheless, this will be done at present; the result will then be subject to corrections which, as we shall show, are small.

Two classes of ^1P states are to be considered: (1) those in which the center of mass of the two neutrons moves with a unit of angular momentum relative to the center of mass of the two protons; (2) the states in which one pair of particles is unexcited while the other is in a P state. A representative of the first class is the function

$$\psi_1=\phi_{100}(1)\phi_{000}(2)\phi_{000}(3)$$

while

$$\psi_1'=(\tfrac{1}{2})^{\frac{1}{2}}\phi_{000}(1)[\phi_{100}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{100}(3)]$$

refers to the latter class.[15] Since we are still dealing with singlet states, the spin functions are the same as in the previous work. ψ_1 and ψ_1' do not combine, nor do the variation functions which improve the one, combine with the other. ψ_1 leads to the variational energy

$$H_{11}=\int\psi_1H\psi_1d\tau=4.05(10+\lambda)\sigma$$
$$-4B\left[1-\frac{\lambda}{2(\sigma+1)}\right]r^3-2Cv^3.$$

ψ_1' gives

$$H_{11}'=4.05(6+5\lambda)\sigma$$
$$-2B\left[1+\frac{\lambda}{4(\sigma+1)}\right]r^3-C\left(\frac{1}{\lambda\sigma+1}\right)v^3.$$

The factor 4.05 here is again simply the value of $\hbar^2\tau/2M$ in Mev, and r and v are defined in (14). Both of these expressions are quite similar in dependence on λ and σ; in particular, neither goes below zero for any permitted value of the variation parameters. There is, to be sure, a groove, but no basin in $\lambda-\sigma$ space. Because of this similarity of behavior, ψ_1' was at this point dismissed from further investigation, and attention was concentrated on the changes which would occur in H_{11} if a greater number of functions were included in the variational calculation. The following were chosen for this purpose:

$$\psi_2=(\tfrac{1}{2})^{\frac{1}{2}}\phi_{100}(1)[\phi_{200}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{200}(3)],$$
$$\psi_3=(\tfrac{1}{2})^{\frac{1}{2}}\phi_{100}(1)[\phi_{110}(2)\phi_{000}(3)+\phi_{000}(2)\phi_{110}(3)].$$

To minimize the energy obtained with the use of these functions with respect to both λ and σ independently would entail a great amount of labor; we have therefore permitted ourselves the following plausible short cut. The greatest contribution to the variational energy comes from ψ_1, which has a minimum with respect to λ ("groove") at $\lambda=1$. The position of this mini-

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[15] The symmetrization of ϕ_{100}, as indicated by (7), is here quite unnecessary, but harmless. It was used in this work because the formulae involving these symmetrized functions were already available. Thus ψ_1 really represents a superposition of 3 degenerate P states.

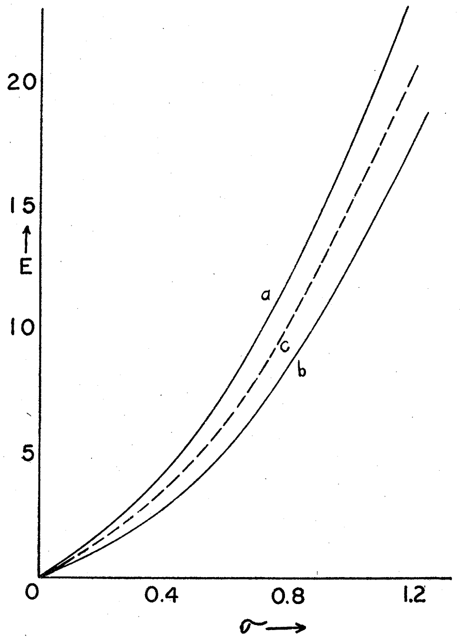

FIG. 3. Energy of ^1P state in Mev, for $\lambda=1$ (groove). a: Variational energy with one function: H_{11}; b: Lowest root of secular equation; c: H_{11} with general Hamiltonian.

mum is not likely to be changed very much by the inclusion of ψ_2 and ψ_3. In the numerical work we shall therefore limit ourselves to this particular value of λ.

The integrations leading to the algebraic form of the matrix elements proceed as before, except that a new set of $r_{ijk,\,lmn}$ has to be calculated. We find

$$H_{22}=4.05(10+5\lambda)\sigma-\frac{5}{2}B\frac{2-\lambda}{\sigma+1}\left[1-2\frac{\sigma+\frac{1}{2}}{\sigma+1}+\frac{\lambda^2}{6}\frac{10\sigma^2+10\sigma+3.5}{(\sigma+1)^2}\right]r^3-2C\left[\frac{\lambda^2\sigma^2+\lambda\sigma+5/4}{(\lambda\sigma+1)^2}\right]v^3,$$

$$H_{33}=4.05(10+5\lambda)\sigma-B\frac{2-\lambda}{\sigma+1}\left[1+\frac{4}{3}\lambda^2\frac{\sigma^2+\sigma+11/16}{(\sigma+1)^2}\right]r^3-2C\left[\frac{\lambda^2\sigma^2+\lambda\sigma+\frac{1}{2}}{(\lambda\sigma+1)^2}\right]v^3,$$

$$H_{12}=-3^{\frac{1}{2}}\left\{8.10\lambda\sigma-B\frac{2-\lambda}{\sigma+1}\left[1-\frac{5}{3}\lambda\frac{\sigma+\frac{1}{2}}{\sigma+1}\right]r^3-C\frac{v^3}{\lambda\sigma+1}\right\},$$

$$H_{13}=-4(\tfrac{1}{6})^{\frac{1}{2}}B(2-\lambda)\frac{\sigma+\frac{1}{2}}{(\sigma+1)^2}r^3,$$

$$H_{23}=-2^{\frac{1}{2}}B\frac{\lambda(2-\lambda)}{\sigma+1}\left[\frac{\sigma+\frac{1}{2}}{\sigma+1}-\frac{\lambda}{3}\frac{5\sigma^2+5\sigma+7/4}{(\sigma+1)^2}\right]r^3.$$

Figure 3 shows H_{11} (upper curve), plotted against σ for the fixed minimizing value of λ. The lower curve represents the root of det $|H_{ij}-E\delta_{ij}|=0$, calculated for different values of σ with the elements given above. Clearly, there is no tendency for the curve to dip below the zero axis, which means that the P state has an energy greater than that of the four dissociated particles composing He^4. It is hardly to be expected that the use of a greater number of functions would change this fact. Such an extension would, however, distort the monotone behavior of the root and presumably produce a minimum somewhere, which would then correspond to the energy of the unstable P state. But it seemed unwise to pursue this matter at present.

The question now arises as to the modification of these results induced by the more general form of the symmetric Hamiltonian. So far, the work was done with the potential energy operator

$$-A\sum\nolimits_1[w+m+\tfrac{1}{2}(b+h)]J_{ij}P_{ij}-A\sum\nolimits_2(w+m-b-h)J_{ij}P_{ij}\quad(15)$$

instead of the correct operator, given by a summation over (1). Since singlet states are symmetric in like particles, the P_{ij} in the second part of (15) are ineffective, so that a correction arises only from the first part. It is thus necessary only to calculate the matrix elements of

$$-A\sum\nolimits_1(w+\tfrac{1}{2}b)J_{ij}(1-P_{ij})\quad(16)$$

and to add them to those found previously. There still exists considerable latitude in the choice of w and b; we will take $w=-2/15$, $b=7/15$. The reason for this selection will be discussed later. The smallness of $(w+b/2)A$ makes it worth while only to compute the effect of (16) on H_{11}, and to neglect it in the secondary contributions to the energy. Now

$$\int\psi_1[\sum\nolimits_1J_{ij}(1-P_{ij})]\psi_1d\tau=4(R_{11}{}^W-R_{11}{}^M),\quad(17)$$

where

$$R_{11}{}^{W}=\frac{(\lambda\sigma+\frac{1}{2})(2-\lambda)}{\lambda(2-\lambda)\sigma+1}\left[\frac{\lambda(2-\lambda)\sigma}{\lambda(2-\lambda)\sigma+1}\right]^{\frac{3}{2}},$$

$$R_{11}{}^{M}=\frac{2-\lambda}{2(\sigma+1)}\left[\frac{\lambda(2-\lambda)\sigma}{\sigma+1}\right]^{\frac{3}{2}}.$$

For $\lambda=1$, (17) is simply $4[\sigma/(\sigma+1)]^{5/2}$, so that the diagonal element of (16) becomes $14.2[\sigma/(\sigma+1)]^{5/2}$. Its addition changes H_{11} of Fig. 3 into the dotted curve drawn below it. The former conclusions are evidently unaltered.

Except for the correction due to (16), the results of this section have already been stated.[16] It was also pointed out in that connection how and why they differ from those obtained by Feenberg[9] and by Bethe and Bacher.[9]

TRIPLET P STATES

The energy of the triplet states depends rather critically on the detailed form of the Hamiltonian. Hence it is advantageous to start with (1) instead of the approximation represented by (3). A triplet function is one in which the spin coordinates of either the two neutrons or the two protons appear symmetrically; hence the coordinate part is antisymmetrical in the chosen pair. In the problem under consideration, the three components of a triplet term coincide because the Hamiltonian here used ignores spin-orbit coupling. We may therefore restrict our investigation for convenience to the state in which $S_z=1$. There will, however, be a doubling of this energy due to neutron-proton symmetry. This appears in Eq. (24).

There are four possible spin functions corresponding to a total spin of one unit along the z-axis. They may be written with an obvious symbolism as follows:

$$\begin{array}{ll} S_1=(+++-), & S_2=(++-+), \\ S_3=(+-++), & S_4=(-+++). \end{array} \qquad (18)$$

From these, two linear combinations can be formed which are symmetric in one pair and antisymmetric in the other. They are, after normalization,

$$(\tfrac{1}{2})^{\frac{1}{2}}(S_3-S_4) \quad \text{and} \quad (\tfrac{1}{2})^{\frac{1}{2}}(S_1-S_2). \qquad (19)$$

(1 and 2, 3 and 4 constitute protons and neutrons respectively, and the signs in the S functions are understood to refer to the particles in this order.)

Now let u be a function of the coordinates, symmetric in 1 and 2, antisymmetric in 3 and 4; and let v be a similar function, but antisymmetric in 1 and 2, symmetric in 3 and 4. A triplet function satisfying the Pauli principle may be written in terms of these as follows:

$$=(\tfrac{1}{2})^{\frac{1}{2}}[au(S_3-S_4)+bv(S_1-S_2)], \qquad (20)$$

where the parameters a and b, which satisfy $a^2+b^2=1$, are to be adjusted for minimum energy.

From (20) we calculate and then minimize

$$\sum_{\sigma}\int \psi H\psi d\tau.$$

The first step is again a summation over the spins, σ. In carrying this out it is to be observed that the only parts of H, Eq. (1), which operate on the spin functions are the Q's, and that these interchange the S functions. Thus, for instance, Q_{12} leaves S_1 and S_2 unchanged, but permutes S_3 and S_4. After the indicated summation we are left with a spin free Hamiltonian, and the problem of minimization affects only the coordinate functions; in fact

$$\sum_{\sigma}\int \psi H\psi d\tau=a^2\int uH_1ud\tau+b^2\int vH_2vd\tau$$
$$+\tfrac{1}{2}ab\left[\int uH_3vd\tau+\int vH_3ud\tau\right]. \qquad (21)$$

The three spin free triplet operators have the form:

$$\begin{aligned} H_1=E_{\text{kin}}-A\textstyle\sum_1[(w+\frac{1}{2}b)+(m+\frac{1}{2}h)P_{ij}]J_{ij} \\ -A[w-b+(m-h)P_{12}]J_{12} \\ -A[w+b+(m+h)P_{34}]J_{34}, \\ H_2=E_{\text{kin}}-A\textstyle\sum_1[(w+\frac{1}{2}b)+(m+\frac{1}{2}h)P_{ij}]J_{ij} \\ -A[w+b+(m+h)P_{12}]J_{12} \\ -A[w-b+(m-h)P_{34}]J_{34}, \\ H_3=-A\{(b+hP_{13})J_{13}-(b+hP_{14})J_{14} \\ +(b+hP_{24})J_{24}-(b+hP_{23})J_{23}\}. \end{aligned} \qquad (22)$$

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[16] H. Margenau, Phys. Rev. **53**, 198 (1938).

It is seen at once that these operators satisfy the relations

$$H_2=P_{13}P_{24}H_1\,;\quad P_{13}P_{24}H_3=H_3. \tag{23}$$

This inherent symmetry shows that the best possible choice which can be made for v is

$$v=P_{13}P_{24}u.$$

From this and Eq. (23) one may deduce:

$$\int vH_2vd\tau=\int(P_{13}P_{24}u)\cdot(P_{13}P_{24}H_1)\cdot(P_{13}P_{24}u)d\tau=\int uH_1ud\tau\,;$$

and similarly

$$\int vH_3ud\tau=\int uH_3vd\tau.$$

If these relations are used, and E is written for the variational energy calculated from (20), Eq. (21) takes the form

$$(a^2+b^2)E=(a^2+b^2)(H_1)_{uu}+ab(H_3)_{uv}.$$

Minimization of E with respect to a and b separately yields the two equations

$$a[(H_1)_{uu}-E]+\tfrac{1}{2}b(H_3)_{uv}=0$$
$$\tfrac{1}{2}a(H_3)_{uv}+b[(H_1)_{uu}-E]=0,$$

which permit nonvanishing solutions for a and b only if the determinant

$$\begin{vmatrix}(H_1)_{uu}-E & \tfrac{1}{2}(H_3)_{uv}\\ \tfrac{1}{2}(H_3)_{uv} & (H_1)_{uu}-E\end{vmatrix}=0.$$

This leads to the energy of the triplet state

$$E=(H_1)_{uu}\pm\tfrac{1}{2}(H_3)_{uv}. \tag{24}$$

In nuclear problems, where present evidence indicates that the spin forces are subordinate to ordinary and Majorana exchange forces, the second term in (24) may be treated as a perturbation. Thus we shall first concentrate our effort upon the problem of choosing a function u which will minimize H_1 regardless of the term $(H_3)_{uv}$.

In line with the general method of this paper, u is taken to be a linear combination of functions of the type $\phi(l_1m_1n_1,1)\phi(l_2m_2n_2,2)\phi(l_3m_3n_3,3)$. The symmetry with respect to permutations of particles required in u may easily be seen to demand that $l_3+m_3+n_3$ be odd, and that the corresponding sums with subscripts 1 and 2 be even. Of course none of the triplet functions combine with the ground state in the present approximation, so that we are again confronted with the problem of finding the lowest possible energy within a given class of variation functions. We must thus look for the lowest root of the resulting secular equation. Since no stable state is likely to result, only two functions have been used in constructing u:

$$\psi_1=\phi_{000}(1)\phi_{000}(2)\phi_{100}(3)$$
$$\psi_2=\phi_{200}(1)\phi_{000}(2)\phi_{100}(3).$$

In view of the symmetry of these functions with respect to P_{12}, and their antisymmetry with respect to P_{34}, one may write, by using (22) and the notation R, S, T, U, V, W previously developed,

$$\begin{aligned}H_1=E_{\text{kin}}+A\{&(m+\tfrac{1}{2}h)(R+S+T+U)^M\\&+(w+\tfrac{1}{2}b)(R+S+T+U)^W\\&+(m+w-b-h)V^M+(m+h-w-b)W^M\}.\end{aligned}$$

The matrix elements for R, S, T, and U are equal; there results, on calculation of R_{11}, V_{11} and W_{11}, the following expression for the diagonal element of H_1 with ψ_1:

$$\begin{aligned}(H_1)_{11}=4.05(6+5\lambda)\sigma&+2A\left\{(m+\tfrac{1}{2}h)\left[1+\tfrac{1}{2}\frac{\lambda}{\sigma+1}\right](r^M)^3+(w+\tfrac{1}{2}b)\left[1+\lambda\frac{\lambda\sigma+\tfrac{1}{2}}{\lambda(2-\lambda)\sigma+1}\right](r^W)^3\right\}\\&+A\left\{(m+w-b-h)+(m+h-w-b)\frac{\lambda\sigma}{\lambda\sigma+1}\right\}v^3.\end{aligned} \tag{25}$$

To carry through the numerical work it becomes necessary to adopt a set of nuclear constants. They may be fixed with a minimum of

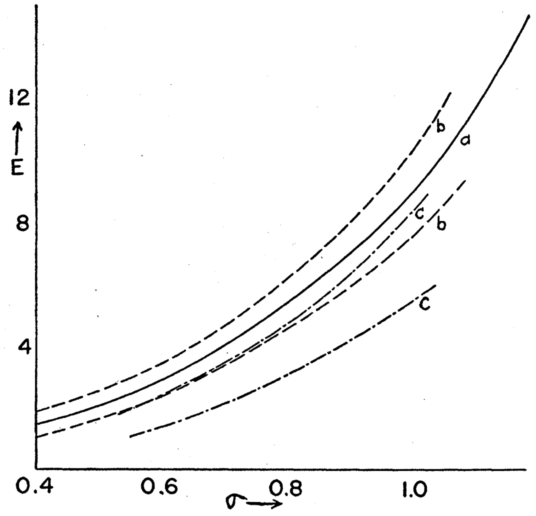

FIG. 4. Energy of ${}^3P$ state in Mev, for $\lambda=0.9$ (groove). a: Variational energy with one function: H_{11}; b: $H_{11} \pm \frac{1}{2}(H_3)uv$; c: Approximate locus of E with inclusion of ψ_2.

uncertainty if we utilize

(a) the fact that $b+h=g$ where g is the parameter determining the triplet-singlet separation of the deuteron levels;
(b) the Breit-Feenberg[11] inequality $m+2h \geqq 4w+2b$;
(c) the Kemmer[17] inequality $m+h \geqq 2w+2b$;
(d) the condition $w+m+b+h=1$.

The value most widely adopted for g is 0.22. We wish to point out that there is considerable uncertainty connected with this choice. As shown previously in this paper, it will not give sufficient binding energy for H^3 and the alpha-particle.[18] For the present let us take a compromise between the customary value and that deduced in an earlier section, and adopt $g=0.20$. As to the inequalities (b) and (c), it was pointed out by Inglis[1] and confirmed by more detailed calculations[19] that the best, though still quite poor, approach to the binding energy of Li^6 is obtainable by taking the equality signs to be valid. This fixes the values to be

$$w=-2/15, \quad m=14/15, \quad b=7/15, \quad h=-4/15.$$

The constant A is of course determined from the theory of the deuteron when the range of the forces is decided upon. As before, A will be taken as 35.6 Mev.

When the expression (25) is evaluated as a function of λ and σ it is found to possess a mild minimum with respect to λ, and this occurs for $\lambda \approx 0.9$. In this groove, however, it is a monotone increasing function of σ. (See Fig. 4, solid curve.) Its behavior is quite similar to that of H_{11} for the ${}^1P$ state.

Neglecting for the moment the effect of ψ_2, we investigate the term splitting due to the second part of (24). We get

$$(H_3)_{uv} = -A\{b(S+U-T-R)^W \\ +h(S+U-T-R)^M\}_{uv}.$$

In the present case, $-S=-U=T=R$ for both Wigner and Majorana forces, so that

$$(H_3)_{uv} = \frac{28}{15} A R_{uv}{}^W - \frac{16}{15} A R_{uv}{}^M.$$

Furthermore,

$$R_{uv}{}^W = \tfrac{1}{2}\left\{\lambda \frac{\lambda\sigma+\frac{1}{2}}{\lambda(2-\lambda)\sigma+1} - 1\right\}(r^W)^3$$

$$R_{uv}{}^M = \tfrac{1}{2}\left\{\frac{\lambda}{4}\,\frac{1}{\sigma+1} - 1\right\}(r^M)^3.$$

The effect of this splitting (for $\lambda=0.9$) is shown by the dotted curves above and below $(H_1)_{11}$ in Fig. 4.

Finally, attention should be given to the effect of the function ψ_2 upon these calculations. For this purpose, $(H_1)_{12}$ has been computed for $\lambda=0.9$ and several values of σ. Only a rough estimate was made of the diagonal element $(H_1)_{22}$; but the accuracy is sufficient to justify the statement that, with the inclusion of ψ_2, the two dotted curves in Fig. 4 would be lowered to an extent indicated approximately by (c). The conclusion, then, is the same as that with regard to the ${}^1P$ state.

Changes in the form of the Hamiltonian would alter these results appreciably. It seems, however, that stability of the P states cannot be brought about by minor adjustments of w, m, b, and h. But an increase in the range of the nuclear forces would make them stable.

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[17] N. Kemmer, Nature **140**, 192 (1937).

[18] The value recently adopted by Heisenberg, Naturwiss. **25**, 749 (1937), $g=0.25$, is even farther from achieving this end.

[19] K. G. Carroll and H. Margenau, Washington Meeting, April 1938, paper 36.