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Perturbation Theory of Light Nuclei: He^4 and Li^6

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Perturbation theory is applied to nuclei in the centrally symmetric representation in which the neutrons and protons have the wave functions of three-dimensional harmonic oscillators. In first order the particles are independent, but the second-order calculation removes this oversimplification. In order to calculate the kinetic energy correctly, a transformation to the coordinate system in which the center of gravity is at rest is introduced. The question of convergence has two aspects: whether the successive contributions, first, of more and more highly excited states, and second, of the successive higher orders, diminish rapidly. One of the many interaction assumptions which are equivalent for He^4 is used in calculating the binding energy of He^4, with a result only slightly less than that given by the equivalent two-body method, a satisfactory proof of both methods. The calculation of the Li^6 binding energy with one form of interaction is carried far enough to include the second-order contribution of the sextuply excited states and the third-order contribution of the doubly excited states, the convergence being apparently sufficiently rapid that further contributions would be negligible. The change in some of the smallest of these contributions effected by altering the interaction assumption is also neglected, in calculating the Li^6 binding energy with other forms of interaction. All forms of interaction considered have a radial dependence resembling the error curve, and all but one treat like-particle and unlike-particle interactions symmetrically. Of these, the only forms which satisfy the demands of scattering and of the H^2 and He^4 energies, and which also give enough binding energy for Li^6, involve combinations of all types of permutation operators with rather large positive and negative coefficients. The influence of the second order on the calculation of nuclear mechanical and magnetic moments, in particular those of Li^6, is also discussed.

METHODS for the calculation of the energies of the two-, three- and four-particle nuclei from assumed interactions of the particles have been developed.[1] With them and from scattering data[2] it has been possible to get valuable indications of the probable approximate nature of the interactions. But the number of accurately known data depending critically on the assumptions is hardly greater than the number of arbitrary constants involved, so that adequate verification of the assumed interactions by prediction of independent results has not been possible. The statistical method (Thomas-Fermi) has been applied to heavy nuclei to test certain assumptions, but has not furnished very definite criteria.[3] It will therefore be important to develop a method for treating the binding and other properties of nuclei consisting of more than four particles.

The success of the perturbation theory in atomic problems[4] suggests a similar attempt in nuclei. The convergence in the atomic case permits no certain prediction of convergence in the nuclear case, for the atom is favored by the

[1] See especially Feenberg and Knipp, Phys. Rev. **48**, 906 (1935); Feenberg and Share, Phys. Rev. **50**, 253 (1936).
[2] As analyzed most recently by Breit, Condon, and Present, Phys. Rev. **50**, 824 (1936).
[3] C. v. Weizsäcker, Zeits. f. Physik **96**, 431 (1935); Breit and Feenberg, Phys. Rev. **50**, 850 (1936); *et al.*
[4] Cf. Condon and Shortley, *Theory of Atomic Spectra* (Cambridge, 1935).

stationary (although, comparing with celestial mechanics, relatively very weak) field of a central particle. In atomic calculations, however, one uses a central field which is, in a Hartree type of approximation, at least directly attributable about as much to the average of the perturbations as to the central particle, and a similar average field enters nuclear calculations also. The manner of carrying out the average, in the atomic case, is strongly influenced by the stabilizing effect of the central particle, and there is no question of disintegration, such as is known in nuclei and might manifest itself as divergence in a calculation with localized wave functions. Formally, in investigating convergence, one has to ask whether integrals H_{ab}, of an interaction multiplied by products of different wave functions of the same variable, are considerably smaller than integrals (or differences of integrals) H_{aa} of a sum of interactions multiplied by squares of wave functions. H_{ab} is reduced by cancellation of positive and negative parts, somewhat more effectively if the interactions vary only slightly within one wavelength, but considerably in any case. H_{aa} is kept within bounds in the atomic case by the screening of the nuclear charge by other electrons, and in nuclei presumably by the exchange nature of the interactions which reduces the effectiveness of the interaction of one particle with many others. The two cases have, then, considerable similarity in the question of expectation of convergence. There are indications that the wave function of a nucleus is not with any accuracy separable into simple, single-particle, wave functions, a sort of complexity which has been discussed in connection with scattering by Bohr,[5] and which one would expect from a naive picture of the problem. There is the alternative picture of a heavy nucleus as a group of alpha-particles intact, but this is probably an over-simplification in the other direction.[6] In cases where an assumption of extreme simplicity has proved satisfactory, as in the Gurney-Condon-Gamow correlation of alpha-emission data, all the simplicity assumed is, of course, not essential to the result. Thus, although one may reasonably hope for convergence, one may also expect that at least the second order of the perturbation theory, which represents a mixing of the simple wave functions of the initially almost independent particles, will be important for some problems.

In selecting a type of initial wave functions with which to calculate, it is essential not only that they bear some resemblance to the true wave functions, but that they lead to integrable expressions when combined with the assumed interactions. At least for light nuclei, with interactions assumed to resemble the Gauss error function, $e^{-\alpha r_{ab}^2}$, both requirements are met in the representation in which each particle is given the wave function of a three-dimensional harmonic oscillator. Since the perturbation theory assumes that the initial wave functions satisfy a zero-order wave equation, we introduce a fictitious zero-order potential

$$V^0 = \tfrac{1}{2}(\sigma\alpha)^2 \Sigma r^2, \tag{1}$$

summed over all particles. Due to the separability of r^2 into x^2, y^2, and z^2, we might use either a Cartesian representation with wave functions separated in Cartesian coordinates, or a spherical representation with wave functions expressed in spherical harmonics. The former seems to be simpler for computing binding energies.

The initial wave functions are still not completely specified, the value of the "inverse-square width" parameter σ being arbitrary. The result of a complete perturbation calculation is expected to converge to the correct energy as rapidly as possible when the initial wave functions are chosen to make the first-order energy as good an approximation as possible. The second-order contribution being negative, the true energy is surely considerably below the first-order energy. We therefore select our initial wave functions by variation of σ for minimum first-order energy. It will be seen, in the cases treated below, that this leads to practically the same second-order energy as does variation of σ for minimum second-order energy.

The center of gravity of all the particles is not at rest in the coordinate system of the wave functions (the oscillations of the individual particles about the origin being independent in zero order, for example). This coordinate system has, then, an irregular "shuttling" motion. The

[5] N. Bohr, Nature, **137**, 344 (1936).
[6] W. Heisenberg, Zeits. f. Physik **96**, 473 (1935).

correct Hamiltonian includes the kinetic energy $\Sigma p'^2/2M$ in a coordinate system x', y', z', in which the laboratory or center of gravity is at rest. For purposes of calculation, this kinetic energy may be expressed in terms of the same coordinates x, y, z, as are the wave functions. We calculate, in a "shuttling" coordinate system for convenience, the average value of the energy in a stationary system (in nonrelativistic approximation). The slight difference between the kinetic energy which we calculate and the kinetic energy of the zeroth order wave equation enters the perturbation procedure just as does the corresponding difference in potential energies, the familiar perturbation term. From $\mathbf{p}'=\mathbf{p}-\Sigma\mathbf{p}/N$, N being the number of particles of equal mass M, we have the wave equation

$$(E-H)\psi=\left\{\frac{1}{2}\left(1-\frac{1}{N}\right)\sum_a\nabla_a^2-\frac{1}{N}\sum_{a>b}\nabla_a\cdot\nabla_b+U-V+E\right\}\psi=0. \quad (2)$$

Here $-U$ is the total binding-type interaction between all particles and V is the Coulomb potential of the protons. The units used (as in Feenberg's papers, from which we shall take parameters) are mc^2 for energy (0.51 Mev) and, to eliminate this and the factor $\hbar^2/M$ from the kinetic energy terms, $\hbar c^{-1}(mM)^{-\frac{1}{2}}$ for length (8.97×10^{-13} cm). In these units the Coulomb energy is

$$V=\frac{\sqrt{1840}}{137}\sum\frac{1}{r}=\frac{\sqrt{2\pi}}{8}\sum\frac{1}{r},$$

summed over proton pairs. The perturbation term in the Hamiltonian is

$$H'=H-H^0=\frac{1}{2N}\sum_a\nabla_a^2+\frac{1}{N}\sum_{a>b}\nabla_a\cdot\nabla_b-U+V-\tfrac{1}{2}(\sigma\alpha)^2\sum_a r_a^2. \quad (3)$$

Although the perturbation potential is not small (V^0 being zero, and $-U$, as we shall specify it, having its deepest negative value when all the coordinates are zero) the effective "perturbing force" is rather small: Considered as functions of one r for example, averaged over the others, $-U$ and V^0 have roughly a constant difference in the region where the wave functions are large, and a constant in H' does not affect the calculations, because of orthogonality. (The rapidly increasing perturbation at large distances, the term V^0, does introduce a tendency for the calculation to diverge in nuclei, but it may be more than compensated, in the comparison with atoms, by the fact that V^0 also keeps the degenerate sets of highly excited levels relatively farther apart than they are in atoms.)

The zero-order wave equation is

$$(E^0-H^0)\psi^0=\{\tfrac{1}{2}\sum_a[\nabla_a^2-(\sigma\alpha)^2r_a^2]+E^0\}\psi^0=0. \quad (4)$$

Using the variables $\xi=(\sigma\alpha)^{\frac{1}{2}}x$, $\eta=(\sigma\alpha)^{\frac{1}{2}}y$, $\zeta=(\sigma\alpha)^{\frac{1}{2}}z$, it has the "Cartesian" solutions

$$\psi^{00}=\prod_{a=1}^{N}\prod_{\xi\eta\zeta}H_{n\xi a}(\xi_a)e^{-\xi_a^2/2} \quad (5)$$

simply products of harmonic oscillator wave functions, wherein we normalize the Hermite polynomials thus:

$$\begin{aligned}
&H_0(\xi)=\pi^{-\frac{1}{4}}, \quad H_1(\xi)=2^{\frac{1}{2}}\pi^{-\frac{1}{4}}\xi,\\
&H_2(\xi)=2^{-\frac{1}{2}}\pi^{-\frac{1}{4}}(2\xi^2-1),\\
&H_3(\xi)=3^{-\frac{1}{2}}\pi^{-\frac{1}{4}}(2\xi^3-3\xi),\\
&H_4(\xi)=2^{-1}6^{-\frac{1}{2}}\pi^{-\frac{1}{4}}(4\xi^4+12\xi^2+3),\\
&H_5(\xi)=2^{-1}15^{-\frac{1}{2}}\pi^{-\frac{1}{4}}(4\xi^5-20\xi^3+15\xi),\\
&H_6(\xi)=12^{-1}15^{-\frac{1}{2}}\pi^{-\frac{1}{4}}(8\xi^6-60\xi^4+90\xi^2-15).
\end{aligned} \quad (6)$$

The zero-order energies are

$$E^0=E_0{}^0+\sum_{\xi,\,a}n_{\xi a}\sigma\alpha.$$

It is convenient to introduce antisymmetry immediately by forming

$$\psi^0=(N_\nu N_\pi)^{-\frac{1}{2}}\sum_{P_\nu P_\pi}(-)^{(P_\nu+P_\pi)}P_\nu P_\pi\psi^{00}\prod_{a=1}^{N}\delta_{m_s a}(\sigma_a), \quad (7)$$

where P_ν is an operator permuting coordinates (including spin) of the N_ν neutrons, and P_π, of the N_π protons, and P in the exponent is the order of the permutation P. $\delta_{m_s a}(\sigma_a)$ is of course a Pauli spin wave function. The usual high degree of degeneracy is apparent. It is only in such cases as the ground states of the alpha-particle, wherein two protons and two neutrons each have three n's equal to zero, or of O^{16}, having as many particles as possible with no n greater than 1,

that there is no degeneracy. The perturbation may be diagonalized within a degenerate set, yielding wave functions ϕ which are linear combinations of the ψ^0's within a degenerate set and which approximate the proper functions of the perturbed system. The first-order energies are then $E^{(1)}=\int\phi H\phi$. In deriving an expression for the second order energies $E^{(2)}$ it is usual to seek ψ expanded in terms of all the ϕ's, which gives $E^{(2)}$ in terms of integrals $\int\phi_a H'\phi_b$. But the degree of degeneracy of the excited states of nuclei is sufficiently high that the selection of the ϕ's may become quite involved. This may be avoided, however, in calculating properties of a state arising from the lowest degenerate set, for example, by expanding ψ in terms of the ϕ's of that set and the ψ^0's of all other sets. The second-order energy is then expressed in terms of integrals $H_{ab}'=\int\phi_a H'\psi_b^0$ thus:

$$E_a^{(2)}=\sum_b (H_{ab}')^2/(E_a^0-E_b^0).$$

The evaluation of the integrals is, of course, unaltered and considerably simplified if one omits the antisymmetry from either ϕ_a or ψ_b^0, modifying the normalization accordingly. The third-order term in the energy is

$$E^{(3)}=\sum_a{}'\sum_b{}'\frac{H_{0a}'(H_{ab}'-\delta_{ab}H_{00}')H_{b0}'}{(E_0-E_a)(E_0-E_b)}. \quad (8)$$

The quadratic array of matrix elements involved makes the computation of $E^{(3)}$ impracticable when many excited states must be taken into account. But an estimate using a limited number of the lower excited states will serve as an indication of the rate of convergence of the method in individual cases.

Types of Interaction

For a preliminary explanation of the trend of the mass defect curve within the limits of accuracy of the statistical model[7] and also for reconciling the mass defects of the deuteron and alpha-particle[8] (with very narrow wave functions), the assumption of binding-type interactions between unlike particles only was sufficient. But the greater stability of even numbers of protons and of neutrons[9] and, recently and more directly, the scattering of protons on protons,[10] indicate the existence of like-particle binding interactions. The proton-proton and neutron-neutron binding interactions are presumably the same, but the former has superposed on it the Coulomb repulsion. Since the like-particle interaction is to be taken of the same order of magnitude as the proton-neutron interaction, it must also be mostly of an exchange nature to avoid collapse of a heavy nucleus. One interaction assumption that satisfies these demands is that used by Feenberg and Knipp:[1]

$$U=B\sum_{\substack{\text{proton-neutron}\\ \text{pairs, ab}}} e^{-\alpha r_{ab}^2}\{(1-g)P_{ab}{}^{(q)}+gP_{ab}\} +C\sum_{\substack{\text{like-particle}\\ \text{pairs, ab}}} e^{-\alpha r_{ab}^2}\frac{2P_{ab}{}^{(q)}+1}{3}. \quad (9_u)$$

The permutation $P^{(q)}$ operates[7] only on space coordinates; P is the more familiar permutation which operates on spin coordinates also.[7] It happens that the values of the parameters B, C and g chosen to fit the neutron-proton and proton-proton scattering data and the binding of the lightest nuclei by the equivalent two-body method[11] are of such a magnitude as to suggest that a simpler interaction is equivalent to (9_u) in problems concerning the ground states of three- and four-particle nuclei.[1] It is

$$U=B\sum_{\text{all pairs}} e^{-\alpha r_{ab}^2}\{(1-g)P_{ab}{}^{(q)}+gP_{ab}\}. \quad (9_s)$$

This interaction is *formally* the same between like and unlike particles, so we may call it a symmetric form of interaction (in contrast with (9_u), which is unsymmetric). It is in effect weaker between like particles than between unlike particles because of the antisymmetry of the wave function in like particles; in the nuclei mentioned, the pairs of like particles have opposite spin, and between them the term in $+gP$ enters only in the "exchange integral," which has a negative sign and is otherwise the same as the direct integral when the ground state of a three- or four-particle nucleus is involved. This with the factor $(1-g)$ in the direct integral makes the effective depth of like-particle interaction

[7] W. Heisenberg, Zeits. f. Physik **77**, 1; **78**, 156; **80**, 587 (1932); E. Majorana, Zeits. f. Physik **82**, 137 (1933).
[8] E. Wigner, Phys. Rev. **48**, 252 (1933).
[9] L. A. Young, Phys. Rev. **48**, 913 (1935); Guggenheimer, J. de phys. et rad. **5**, 475 (1934).
[10] Tuve, Heydenberg and Hafstad, Phys. Rev. **50**, 806 (1936).
[11] E. Feenberg, Phys. Rev. **47**, 850 (1935); Feenberg and Knipp, reference 1.

$(1-2g)B$. If this is equal to C, (9_u) and (9_s) are equivalent in these nuclei. It is apparent that the same equivalence does not exist for heavier nuclei, so we shall be able to decide which type of interaction is more nearly satisfactory. Finding neither adequate, we shall also consider other types (Eq. (17)).

Integration

In the calculation of matrices of these interactions, we encounter integrations of the type $\int \psi_g^{00} U \psi_k^{00} d\tau_1 \cdots d\tau_N$. Because of the separability of such integrals in Cartesian coordinates and the absence of more-than-two-particle interactions, they reduce to products of integrals which we designate thus:

$$f_{abcd}=(\tau/\sigma)^{\frac{1}{2}}\int_{-\infty}^{\infty} H_a(\xi)H_b(\chi) \times e^{-\{\xi^2+\chi^2+(\xi-\chi)^2/\sigma\}}H_c(\xi)H_d(\chi)d\xi d\chi$$

$$=(\tau/\sigma)^{\frac{1}{2}}\int_{-\infty}^{\infty} d\xi H_a(\xi)H_c(\xi)e^{-\xi^2\tau/(\sigma+1)} \times\int_{-\infty}^{\infty} d\nu H_b(\xi/(\sigma+1)+\nu) \times H_d(\xi/(\sigma+1)+\nu)e^{\nu^2(\sigma+1)/\sigma},$$

where $\tau=\sigma+2$. We note that $f_{abcd}=f_{adcb}=f_{cbad}$. Instead of writing a closed form for these, which would, it seems, be rather intricate, we find it convenient to list the integrals which we shall need in subsequent calculations:

$$\begin{aligned}
&f_{0000}=1,\\
&f_{1100}=1/\tau,\\
&f_{1010}=1-1/\tau,\\
&f_{2000}=-1/(2^{\frac{1}{2}}\tau),\\
&f_{1111}=1-2/\tau+3/\tau^2\\
&f_{2110}=(2/\tau-3/\tau^2)/2^{\frac{1}{2}},\\
&f_{2101}=(-1/\tau+3/\tau^2)/2^{\frac{1}{2}},\\
&f_{2200}=3/(2\tau^2),\\
&f_{2020}=1-2/\tau^2+(3/2)/\tau^2,\\
&f_{3100}=-(3/2)^{\frac{1}{2}}/\tau^2,\\
&f_{3010}=(3/2)^{\frac{1}{2}}(-1/\tau+1/\tau^2),\\
&f_{4000}=(3/2)^{\frac{1}{2}}/(2\tau^2),\\
&f_{2211}=2/\tau-6/\tau^2+(15/2)/\tau^3,\\
&f_{3111}=(3/2)^{\frac{1}{2}}(-1/\tau+4/\tau^2-5/\tau^3),\\
&f_{3210}=(3^{\frac{1}{2}}/2)(3/\tau^2-5/\tau^3),\\
&f_{3201}=3^{\frac{1}{2}}(-1/\tau^2+(5/2)/\tau^3),\\
&f_{3300}=5/(2\tau^3),\\
&f_{4110}=(3/2)^{\frac{1}{2}}(-2/\tau^2+(5/2)/\tau^3),\\
&f_{4101}=(3/8)^{\frac{1}{2}}(1/\tau^2-5/\tau^3),\\
&f_{4200}=-3^{\frac{1}{2}}5/(4\tau^3),\\
&f_{5100}=(15/8)^{\frac{1}{2}}/\tau^3,\\
&f_{6000}=-5^{\frac{1}{2}}/(4\tau^3).
\end{aligned}\tag{10}$$

The Binding Energy of the Alpha-Particle

An impression of the extent and convergence of the perturbation calculation can be had by examination of the details of this example, using, explicitly, the unsymmetrical form of interaction.[12] A zero-order state of the alpha-particle can be described in all detail by giving sixteen quantum numbers, describing the x, y, and z oscillations and the spin of each particle. For a certain excited state, we have for example the list 100+, 000−; 000+, 100− where the numbers give n's and the signs give the sign of m_s, those before the semicolon (;) referring to neutrons and the others to protons. This can be abbreviated 1, 0; 0, 1 if omitted n_η's and n_ξ's are understood to be zero and + is understood to come before −. In calculating the diagonal energy for a state, the symmetry between the particles and the separability into x, y, and z integrals, reduces the integration to simple forms. For example, for the ground state, 0, 0; 0, 0, we have

$$(0,0;0,0|\Sigma\nabla_a^2|0,0;0,0) =12(0|d^2/dx^2|0)=-6\sigma\alpha.$$

The terms in $\nabla_a\cdot\nabla_b$ here give nothing, being products of odd functions of different variables. The average binding potential is

$$\begin{aligned}(0,0;0,0|U|0,0;0,0)&=\{(4-2g)B+2C\}(0,0|e^{-\alpha x^2_{ab}}|0,0)\\&=\{(4-2g)B+2C\}(\sigma/\tau)^{\frac{3}{2}}.\end{aligned}$$

The Coulomb term is reduced by a factor 1/2 because of exchange, leaving[6] $(\alpha\sigma)^{\frac{1}{2}}/4$. We have, then, for the first-order energy of the alpha-particle,

$$E^{(0)}+E^{(1)}=(9/4)\alpha\sigma -2\{(2-g)B+C\}(\sigma/\tau)^{\frac{3}{2}}+(\alpha\sigma)^{\frac{1}{2}}/4. \quad (11)$$

The second-order energy consists of contributions from many excited states. The integrals H_{oa}' are zero between the ground state and any excited states for which the sum of the n's is an odd number, because H' is odd in an even number of coordinates and the wave function is odd in an odd number of coordinates. The states of the

[12] Preliminary results for the still simpler case of unlike-particle interactions only were given in an abstract: Inglis, Phys. Rev. **50**, 399. More accurate calculation shows those results to be about two percent low. The first order only was given by Heisenberg, reference 6.

TABLE I. *Doubly excited states of He⁴.*

TYPE	NR.	H_{oa}'	H_{oa}' ($\sigma=2.6$, etc.)
$+\ -\ +\ -$			
2, 0; 0, 0	12	$\{(2-g)B+C)u/\tau-3\alpha\sigma/8\}/\sqrt{2}$	−0.19
1, 0; 1, 0	6	$-Bu/\tau+\alpha\sigma/8$	−1.45
1, 0; 0, 1	6	$-(1-g)Bu/\tau+\alpha\sigma/8$	−0.09
1, 1; 0, 0	6	$-Cu/\tau+\alpha\sigma/8$	1.27
$+\ +\ -\ -$			
0, 1; 1, 0	3	$-gBu/\tau$	−1.36

system which do contribute to the second order may then be grouped as doubly excited states (degenerate with $E_a^0=E_o^0+2\alpha\sigma$), quadruply excited states, sextuply excited states, etc. Of these, only those with Σn_ξ, Σn_η, and Σn_ζ separately equal to even integers have nonvanishing nondiagonal elements H_{oa}'. The number of contributing states is further limited by the fact that no term in the Hamiltonian involves more than two particles, so only one or two particles may be excited in a contributing state, and by the selection rule $\Delta M_S=0$ which confines our attention to one value of total spin projection, because our operators in this approximation introduce no spin-orbit coupling. The Coulomb term is for light nuclei very much smaller than the rest of the Hamiltonian, so we neglect it beyond the first order, which leaves H' symmetrical with respect to protons and neutrons. Because of the equivalence of the particles and of directions in space, there are several doubly excited states of the same type, having the same value of H_{oa}'. The number of states of one type is the product of the number of permutations of its set of n's in x, y, and z, multiplied by two if protons and neutrons are not excited symmetrically, and again multiplied by two if the excitation is not symmetrical relative to + and −. The types of states, with the number of states of each type and the corresponding expressions for H_{oa} in terms of the parameters, are given in Table I. The sequence of m_s is the same as for the ground state, except for the last line, as indicated. For brevity, we introduce $u=(\sigma/\tau)^{\frac{3}{2}}=(\sigma/(\sigma+2))^{\frac{3}{2}}$. Terms in $\alpha\sigma$ do not occur in H_{oa}' beyond the doubly excited states (cf. the selection rule for the harmonic oscillator) The third, fourth, and fifth types listed in Table I have matrix elements H_{oa}' quite similar to that of the second type, differing, aside from the terms in $\alpha\sigma$, in the replacement of B by $(1-g)B$, C, and gB, respectively. The same similarity recurs through the higher states, and we shall shorten the tables by listing only one of the four similar types explicitly and indicating the omission by an asterisk (*). With this understanding, the types of quadruply and sextuply excited states are indicated in Table II. In order to be able to compare the contributions of the various groups of states, we shall split the second-order term in the energy of the ground state into a part due to all doubly excited states, a part due to all quadruply excited states, etc., thus: $E^{(2)}=E_D{}^{(2)}+E_Q{}^{(2)}+E_S{}^{(2)}+\cdots$. Adding the contributions from the types of states listed in Tables I and II, we have

$$-E_D{}^{(2)}=3\{(F+G)u^2/(\tau^2\alpha\sigma)-[(2-g)B+C]u/\tau+3\alpha\sigma/16,$$

$$-E_Q{}^{(2)}=3(31F+5G)u^2/(8\tau^4\alpha\sigma),$$

$$-E_S{}^{(2)}=(815F+33G)u^2/(24\tau^6\alpha\sigma),$$

where

$$F=2(1-g+3g^2/4)B^2+C^2$$

and

$$G=[(2-g)B+C]^2.$$

Now we are in a position to obtain a numerical second-order result for the binding energy by assuming values of the parameters α, g, B, and C. It has been stated that the unsymmetrical form of interaction (9_u) and the symmetrical form (9_s)

TABLE II. *Quadruply and sextuply excited states of He⁴.*

TYPE a				NR.	$(\tau^2/u)H_{oa}'$
+	−	+	−		
4,	0;	0,	0	12	$(3/8)^{\frac{1}{2}}\{(2-g)B+C\}$
22,	0;	0,	0	12	$-(1/2)\{(2-g)B+C\}$
3,	0;	1,	0	12*	$(3/2)^{\frac{1}{2}}B$
12,	0;	1,	0	12*	$(1/2)^{\frac{1}{2}}B$
2,	0;	2,	0	6*	$-(3/2)B$
2,	0;	02,	0	12*	$-(1/2)B$
11,	0;	11,	0	6*	$-B$
6,	0;	0,	0	12	$(5^{\frac{1}{2}}/4)\{(2-g)B+C\}/\tau$
42,	0;	0,	0	24	$(3^{\frac{1}{2}}/4)\{(2-g)B+C\}/\tau$
222,	0;	0,	0	4	$(1/2)^{\frac{3}{2}}\{(2-g)B+C\}/\tau$
5,	0;	1,	0	12*	$(15/8)^{\frac{1}{2}}B/\tau$
32,	0;	1,	0	24*	$-(3^{\frac{1}{2}}/2)B/\tau$
122,	0;	1,	0	12*	$-(1/2)B/\tau$
4,	0;	2,	0	12*	$-(5/4)3^{\frac{1}{2}}B/\tau$
4,	0;	02,	0	24*	$(3^{\frac{1}{2}}/4)B/\tau$
22,	0;	2,	0	24*	$3(1/2)^{\frac{1}{2}}B/\tau$
022,	0;	2,	0	12*	$(1/2)^{\frac{1}{2}}B/\tau$
112,	0;	11,	0	12*	$(1/2)^{\frac{1}{2}}B/\tau$
3,	0;	3,	0	6*	$(5/2)B/\tau$
3,	0;	12,	0	24*	$-(3^{\frac{1}{2}}/2)B/\tau$
21,	0;	21,	0	12*	$-(3/2)B/\tau$
012,	0;	21,	0	12*	$-(1/2)B/\tau$
111,	0;	111,	0	2*	$-B/\tau$

are approximately equivalent, with the values of the parameters found by Feenberg and Knipp. We shall alter those values very slightly, so as to make the two forms of interaction exactly equivalent in this calculation, while altering the results very little, by taking $\alpha=16$, $B=72$, $C=42.5$, $g=0.205$. (With these values, the equivalent two-body method gives the binding energy of the alpha-particle $-E=56mc^2$. The values of α and B were kindly suggested by Dr. Feenberg, as better fitting newer mass determinations.) In varying σ for minimum (first-order) energy, numerically, it is more instructive, and somewhat easier, to calculate energies directly than to use the equation for the derivative. In Table III are given values of the separate terms in the energy, calculated in units mc^2 with these parameters, for values of σ about the minimum. From these values it is apparent that it makes practically no difference in the second-order energy, whether we vary σ for minimum first-order energy and calculate the second-order term with the value of σ so determined, or vary σ for minimum second-order energy directly. The most striking feature of the results given is that the quadruply excited states contribute much more than the doubly excited states. This does not mean, however, that the calculation will not converge, since there is a good reason for this exception to the expected rule that each group should contribute much less than the preceding group. The reason is that the terms in $\alpha\sigma$, which are found for the doubly excited states only (see Table I), enter the matrix elements with opposite sign to that of B or C, and greatly reduce their values. (The value of $-E_D^{(2)}$ listed for $\sigma=2.6$ is calculated as $44.8-44.5=0.3$, for example.) So the convergence does not seem to commence until after the quadruply excited states. We take the small value of $E_S^{(2)}$ as sufficient indication that we have quite a good value ($-E^{(1)}-E^{(2)}=53.0mc^2$) of the second-order binding energy without proceeding further.

The third-order term in the energy (8) is laborious to calculate, so we shall not make as careful an estimate of it as we have made of the second-order, and shall do it only for our present choice of parameters and for $\sigma=2.6$. First we confine our attention to the doubly excited states, and evaluate the elements H_{oa}' for them,

TABLE III. *Terms of the second-order binding energy of He^4 (in units mc^2) for values of σ about the minimum.*

σ	2.4	2.5	2.6	2.7	2.8
$-E^{(1)}$	50.4	50.7	50.8	50.7	50.5
$-E_D^{(2)}$	0.1		0.3		0.6
$-E_Q^{(2)}$	2.0		1.7		1.5
$-E_S^{(2)}$	0.2_3		0.1_9		0.1_4

as entered in the last column of Table I. Examining these numbers, we see that we may, as an approximation, neglect the first and third types. The second, fourth, and fifth types have, respectively, the following values of the expression $H_{aa}'-H_{oo}'$ which enters (8):

$$1,\ 0;\ 1,\ 0:\ [2(1-g)-g/\tau+3/\tau^2]B+2(1-1/\tau)Cu-5\alpha\sigma/4=136mc^2,$$

$$1,\ 1;\ 0,\ 0:\ \{2(2-g)(1-1/\tau)B-(2-3/\tau)C/\tau\}u-5\alpha\sigma/4=138mc^2,$$

$$1^+,\ 0^+;\ 1^-,\ 0^-:\ \{[2(2-g)(1-2/\tau)-3/\tau^2]B+2[1+1/(3\tau)]C\}u-3\alpha\sigma/2=99mc^2.$$

The nondiagonal element H_{ab}' between the first two of the states here listed is $(\sigma+1)Bu/\tau=24mc^2$; all other nondiagonal elements between these types of states, or between states of the same type, are smaller at least by a factor g or $1/\tau$ (and are not all of the same sign), so we may neglect them. Substituting these values and those of Table I in (8), enumerating the states of each type, and remembering that the "nondiagonal" terms enter twice because the two summations in (8) are independent, we have for the part of the third-order term in the energy due to doubly excited states only:

$$E_D^{(3)}\approx 0.5_6mc^2.$$

Of this about $-0.04mc^2$ is due to the "nondiagonal" terms. A rough estimate of the total contribution to (8) of all terms involving both doubly and quadruply excited states is $-0.01mc^2$. The "nondiagonal" terms being apparently negligible, we estimate further only the "diagonal" terms of the quadruply excited states, and find roughly

$$E_Q^{(3)}\approx -0.0_5mc^2,$$

the principal contributions ($-0.1mc^2$) coming from the types 4, 0; 0, 0 and 22, 0; 0, 0. The result is at least accurate enough to show that, contrary to the situation in the second order,

the third-order contribution of the quadruply excited states is considerably smaller than that of the doubly excited states. $E_Q^{(3)}$ is also much less than $E_Q^{(2)}$, which seems to indicate that the convergence is rapid.

Combining the various terms, we have for the binding energy of the alpha-particle, as calculated with our choice of parameters, $-E=52.5mc^2$. The same parameters give $56mc^2$ by the equivalent two-body method, which probably indicates an upper limit.[1] Considering the binding energy as the difference between an average potential and an average kinetic energy, the agreement is really quite close, and the slight difference between the calculated binding energy $52.5mc^2$ and the observed value $55mc^2$ indicates that the parameters probably should be readjusted slightly.

The Binding Energy of Li^6

A calculation of the binding energy of Li^6 is complicated, compared to the above, by the degeneracy of the lowest states in zeroth order. The first-order calculation consists of selecting a linear combination of those states in such a way as to diagonalize the submatrix of the energy between them. There are no matrix elements between states with different total projection of spin angular momentum, because the operators in (9) do no more than interchange spin coordinates, without changing their sum. We therefore have small submatrices for $M_S=1$ and for $M_S=0$. The neglect of spin-orbit coupling further means that the total spin and total orbital angular momentum separately commute with the Hamiltonian, as in atomic spectra, so that the states with diagonalized energy are also characterized by the quantum numbers L and S of Russell-Saunders coupling. The same first-order result has been obtained independently by Feenberg and Wigner[13] and by Bethe and Rose,[14] by first diagonalizing the angular momenta and then calculating the energy in terms of certain parameters, for Li^6 and other light nuclei. The diagonalization of the energy may be carried out directly for Li^6. The energy may also be had from the secular problem with our wave functions, as we shall now show.

[13] Feenberg and Wigner, Phys. Rev. **51**, 95 (1937).
[14] Bethe and Rose, Phys. Rev. **51**, 283 (1937).

The nine states with $M_S=1$ may be grouped, according to their four small submatrices of the interaction, thus: (1; 1), (01; 01), (001; 001) with a three-row matrix, and the pair (1; 01), (01; 1) having the same submatrix as has the pair (1; 001), (001; 1) and the pair (01; 001), (001; 01), all of which may be seen from symmetry. After subtracting (0, 0, 1; 0, 0, 1|H|0, 0, 1; 0, 0, 1) from the diagonal elements, the submatrices are

$$\begin{vmatrix} 0 & -a & -a \\ -a & 0 & -a \\ -a & -a & 0 \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} b & -d \\ -d & b \end{vmatrix} \tag{13}$$

where $a=Bf^2_{1100}$, $b=B(f_{1111}-f^2_{1100})$, and $d=Bf^2_{1010}$, using either of the forms of interaction (9). The three consequent two-row secular determinants each have the roots $b+d$, and $b-d=a$, using (10). The three-row secular determinant is easily factored by adding rows and subtracting columns, yielding the roots a, a, $-2a$. The fivefold root a corresponds of course to the energy of the ^3D, $b+d$ to ^3P, and the lowest root $-2a$ to the ^3S. The latter root in the three-term secular equations leads to the wave function

$$\phi_0=3^{-\frac{1}{2}}\{(1;1)+(01;01)+(001;001)\}. \tag{14}$$

This is the ground state, since the interactions have been chosen to make triplets lie below singlets in cases like this and the deuteron, where essentially only one proton-neutron interaction is involved.

The energies of the singlets may be had explicitly by considering the states with $M_S=0$, which fall into groups twice as large as those just considered. The ^1D and ^1P are had as $\{f_{1111}-(1-2g)(f^2_{1100}\pm f^2_{1010})\}B$ from one of the four-row submatrices (factoring by adding rows and subtracting columns in blocks of two) and the ^1S as $\{-2f_{1111}+(1-2g)(f^2_{1010}-f^2_{1001})\}B$ from the trace ($=0$) of the six-row submatrix, knowing the other terms, and using the sum rule

The ground state has, then, the first-order energy (0, 0, 1; 0, 0, 1|H|0, 0, 1; 0, 0, 1)$-2a$. Using the symmetrical form of interaction (9_s), this is[15]

$$E^{(0)}+E^{(1)}=55\alpha\sigma/12-\{5-8g+(8-2g)/\tau+5/\tau^2\}uB+0.7(\alpha\sigma)^{\frac{1}{2}}. \tag{15$_s$}$$

[15] The Coulomb energy is calculated here to first order, and roughly for other nuclei from He to O having $2+\lambda$ protons, by taking (reference 6) $\rho(r,r')=2(\alpha\sigma/\pi)^{3/2}(1+\alpha\sigma\lambda r\cdot r'/3)e^{-\alpha\sigma(r^2+r'^2)/2}$, to be $(2+3\lambda+43\lambda^2/72)(\alpha\sigma)^{\frac{1}{2}}/8$.

Using the unsymmetrical form (9_u), we have instead

$$E^{(0)}+E^{(1)}=55\alpha\sigma/12-\{[5-2g+2(3-g)/\tau+5/\tau^2]B+2(1+1/\tau)C\}u+0.7(\alpha\sigma)^{\frac{1}{2}}. \quad (15_u)$$

In calculating the second-order contribution to the energy of the ground state, we may again group the doubly excited states, for example, in types such that all states of the same type have the same value of H_{oa}'. This follows from the isotropic nature of the wave function of the ground state (14), which means that exchange of directions, as well as exchange of all protons with all neutrons, in the description of the excited state, does not alter the integral. As an illustration of the difference between this calculation and that of the alpha-particle, which has been given in detail, we list in Table IV the types of doubly-excited states which we take into account. The matrix elements H_{oa}' are listed in a general form for future reference, and they are reduced to the matrix elements of our present calculation by putting $g_1=g_\sigma=0$.

Adding the squares of the matrix elements of these states, and dividing by $2\alpha\sigma$, we get their contribution to the second-order term in the energy:

$$E_D^{(2)}=-\{52-62g+59g^2-(70+40g+10g^2)/\tau+(180-85g+27g^2)/\tau^2-(70+35g)/\tau^3+214/\tau^4\}(Bu/\tau)^2/\alpha\sigma+\{64-126g+(154-60g)/\tau+203/\tau^2\}(Bu/\tau)/12-(323/288)\alpha\sigma. \quad (16_s)$$

The corresponding computation using the unsymmetrical form of interaction (9_u) (for states having both a neutron and a proton excited, the calculation is of course unaltered) gives

$$E_D^{(2)}=-\{[(63-38g+25g^2)\sigma^2+2(91-71g+32g^2)\sigma+237-172g+74g^2+20(2\sigma-1-g)\times(7/2\tau)+35(7/2\tau)^2]B^2+[2(12-20g/3)\sigma^2+(53-85g/3)\sigma+63-40g+35/\tau]BC+[12\sigma^2+48\sigma+63]C^2\}u^2/(2\alpha\sigma\tau^4)+\{[(46-11g)\sigma+89-52g+29(7/2\tau)]B+[38\sigma/3+52]C\}u/(6\tau^2)-323\alpha\sigma/288. \quad (16_u)$$

Using the parameters $\alpha=16$, $B=72$, $C=42.5$, and $g=0.205$, as for the alpha-particle above, we evaluate (15) and (16) for the symmetrical form in Table V and for the unsymmetrical form in Table VI, for values of σ about the minimum. We see that there is here considerable difference in the behavior of the two forms of interaction.

TABLE IV. *Doubly excited states of Li^6.*

TYPE						NR.	$\sqrt{3}H_{oa}'$
+	−	+	+	−	+		
0,	0,	3;	0,	0,	1	6	$(3/2)^{\frac{1}{2}}\{[(-g+5g_1+3g_\sigma)/\tau+(1-g-10g_1-9g_\sigma)/\tau^2+7/\tau^3]\text{Bu}-5\alpha\sigma/12\}$
0,	0,	12;	0,	0,	1	12	$2^{-\frac{1}{2}}\{[(-g+5g_1+3g_\sigma)/\tau+(1-g-10g_1-9g_\sigma)/\tau^2+7/\tau^3]\text{Bu}-5\alpha\sigma/12\}$
2,	0,	1;	0,	0,	1	6	$2^{-\frac{1}{2}}\{[(-2-3g+9g_1+6g_\sigma)/\tau+9(1-2g_1-2g_\sigma)/\tau^2]\text{Bu}-5\alpha\sigma/12\}$
0,	2,	1;	0,	0,	1	6	$2^{-\frac{1}{2}}\{[(-1+6g_1+3g_\sigma)/\tau+3(2-g-4g_1-3g_\sigma)/\tau^2]\text{Bu}-5\alpha\sigma/12\}$
02,	0,	1;	0,	0,	1	12	$2^{-\frac{1}{2}}\{[(2-3g+3g_1)/\tau+3(1-2g_1-2g_\sigma)/\tau^2]\text{Bu}-5\alpha\sigma/12\}$
0,	02,	1;	0,	0,	1	12	$2^{-\frac{1}{2}}\{[(3-4g+2g_1-3g_\sigma)/\tau+(2-g-4g_1-3g_\sigma)/\tau^2]\text{Bu}-5\alpha\sigma/12\}$
11,	0,	1;	0,	0,	01	12	$[(-2+3g_1+3g_\sigma)/\tau+3(1-2g_1-2g_\sigma)/\tau^2]\text{Bu}$
0,	11,	1;	0,	0,	01	12	$[(-2+2g+2g_1+3g_\sigma)/\tau+(2-g-4g_1-3g_\sigma)/\tau^2]\text{Bu}$
0,	0,	2;	0,	0,	2	3	$\{[-2/\tau+6/\tau^2-21/(2\tau^3)]\text{Bu}+\alpha\sigma/6\}$
0,	0,	11;	0,	0,	11	3	$\{[-2/\tau+4/\tau^2-7/\tau^3]\text{Bu}+\alpha\sigma/12\}$
0,	0,	2;	0,	0,	02	6	$2/\tau^2-7/(2\tau^3)\text{Bu}$
0,	1,	1;	0,	0,	2	6	$2^{-\frac{1}{2}}\{[(1-g-3g_1-g_\sigma)/\tau+3(-1+g+2g_1+g_\sigma)/\tau^2]\text{Bu}+\alpha\sigma/6\}$
0,	1,	1;	0,	0,	02	12	$2^{-\frac{1}{2}}\{(1-g-g_1-g_\sigma)/\tau+(-1+g+2g_1+g_\sigma)/\tau^2\}\text{Bu}$
01,	0,	1;	0,	0,	11	6	0
0,	01,	1;	0,	0,	11	12	$[-g_1/\tau+(-1+g+2g_1+g_\sigma)/\tau^2]\text{Bu}+\alpha\sigma/12$
01,	0,	1;	01,	0,	1	12	$-2\text{Bu}/\tau+\alpha\sigma/6$
01,	0,	1;	0,	01,	1	12	$(-1+g+g_\sigma)\text{Bu}/\tau+\alpha\sigma/12$
0,	1,	1;	0,	1,	1	9	$-\text{Bu}/\tau+\alpha\sigma/12$
0,	1,	2;	0,	0,	1	6	$2^{-\frac{1}{2}}\{[(1+g-3g_1-2g_\sigma)/\tau+3(-1+2g_1+2g_\sigma)/\tau^2]\text{Bu}+\alpha\sigma/6$
0,	1,	02;	0,	0,	1	12	$2^{-\frac{1}{2}}[(+1-g-g_1-2g_\sigma)/\tau+(-1+2g_1+2g_\sigma)/\tau^2]\text{Bu}$
0,	01,	11;	0,	0,	1	12	$\{(g-g_1)/\tau+(-1+2g_1+2g_\sigma)/\tau^2\}\text{Bu}+\alpha\sigma/12$
01,	01,	1;	0,	0,	1	12	$(-1+2g+2g_\sigma)\text{Bu}/\tau+\alpha\sigma/12$
+	+	+	+	−	−		
0,	2,	1;	0,	0,	1	6	$2^{-\frac{1}{2}}\{(2g-g_\sigma)/\tau-(3g-3g_\sigma)/\tau^2\}\text{Bu}$
0,	02,	1;	0,	0,	1	12	$2^{-\frac{1}{2}}\{g_\sigma/\tau+(g-g_\sigma)/\tau^2\}\text{Bu}$
0,	11,	1;	0,	0,	01	12	$\{-g/\tau+(g-g_\sigma)/\tau^2\}\text{Bu}$
0,	1,	01;	0,	0,	11	12	$\{-g_\sigma/\tau+(-g+g_\sigma)/\tau^2\}\text{Bu}$

TABLE V. *Symmetrical form (Eq. 9_s).*

σ	0.8	1.0	1.2	1.4
$-E^{(0)}-E^{(1)}$	12.6	13.3	12.7	8.7
$-E_D^{(2)}$	19.3	22.1	24.1	25.6

TABLE VI. *Unsymmetrical form (Eq. 9_u).*

σ	1.2	1.4	1.6	1.8
$-E^{(0)}-E^{(1)}$	26.9	27.4	26.9	25.1
$-E_D^{(2)}$	18.1	17.9	17.6	17.5

At least to this order of accuracy, the nucleus seems to be more unstable and larger (smaller σ) with the symmetric form of interaction than with the unsymmetric. This "repulsive" effect of the symmetrical form may be traced to the interaction between like particles with like spins: the entire operator $\{(1-g)P^{(q)}+gP\}$ annuls the exchange nature of the "exchange integral" introduced by antisymmetry, thus augmenting its magnitude without changing its sign.

Comparing these results with those for the alpha-particle, we see that the second-order contribution to the energy is of a *larger order of magnitude* for Li^6. On the other hand, they are both calculated as differences of quantities of the same order of magnitude (the value $-E_D^{(2)}=17.9$ in Table VI is found as $75.6-57.7$ for example; cf. $44.8-44.5=0.3$ for the alpha-particle, in Table III above). This may be interpreted as an illustration of fact that the zero-order potential V^0 can be chosen to fit all the particles in the alpha-particle very well, since they are *equivalent* particles (namely, s-particles), whereas in Li^6 the size of V^0 must be adjusted as a compromise between the tendency of the four s particles to congregate closely and the tendency of the more loosely-bound p particles to spread out. Thus V^0 is not as good an approximation to the true average potential in Li^6, and the correction introduced by the second-order contribution is larger. In more detail, $E_D^{(2)}$ is easily seen to depend essentially upon a mean-square difference between the "U part" and the "V^0 part" of the elements H_{oa}' (the kinetic energy correction also enters here, but in a secondary rôle). This is not true of the further contributions $E_Q^{(2)}$, etc., a selection rule excluding the "V^0 part," as we have seen. Since the positive part of $-E_D^{(2)}$ alone is of the same order of magnitude in Li^6 as in the alpha-particle, we may expect contributions of the quadruply excited states, etc., to be of the same order of magnitude in the two nuclei.

In further investigation of the convergence, the types of quadruply excited states have been listed (but the reader is spared the sight of them!), with the number of states of each type, and a numerical evaluation of the matrix elements H_{oa}', for each form of interaction, and for approximately the value of σ which gives a minimum value to $E^{(0)}+E^{(1)}$. Computation with these elements leads to the following values:

Symmetrical form of U, $\sigma=1$, $\quad -E_Q^{(2)}=6._0mc^2$.

Unsymmetrical form of U, $\sigma=1.4$,
$\quad -E_Q^{(2)}=5._5mc^2$.

To give an idea of the slope of $-E_Q^{(2)}(\sigma)$, the value for the symmetrical form and $\sigma=1.2$ was found to be about $6._4mc^2$. The second-order contribution of the sextuply states we only estimate very roughly, by analogy with the last calculation, by noting that half of the contributions to $-E_Q^{(2)}$ (symmetrical form of U) are made by states in which the s particles alone are excited, and a quarter by the types 04, 0, 1; 0, 0, 1 and 0, 04, 1; 0, 0, 1 and 2, 0, 1; 2, 0, 1 and 2, 0, 1; 0, 2, 1. The six analogous types of sextuply excited states contribute 0.05, and this is apt to be roughly the same fraction of the total (a survey of the details that make one type of state contribute less than another may be necessary to convince one of this), which leads to the estimate $-E_S^{(2)}=0._2$. Experience with the alpha-particle has shown that the "non-diagonal" terms of the summation may be neglected in reckoning the third-order contribution to the energy. Doing this, and proceeding otherwise as for the alpha-particle, we find $-E_D^{(3)}=-1._5$, as calculated with the symmetrical form of interaction. This we take as sufficiently definite indication of rapid convergence. Since the neglected nondiagonal terms are apt to oppose in sign the neglected fourth-order contribution to the energy, we take as our (most probable!) result the sum of the terms we have cited, or

$-E=40._1mc^2$, for the symmetrical form of U

$-E=49._5mc^2$, for the unsymmetrical form.

The approximations made in estimating the contributions of some excited states and neglecting others lead to errors in the result of probably not more than $1mc^2$, in the judgment of the writer.

The parameters here used were essentially those previously determined by the equivalent two-body method. By our method they gave $52.5mc^2$ instead of $55mc^2$ for the binding energy of the alpha-particle. If, in order not to alter the deuteron results, we simply change C to make the alpha binding $55mc^2$ by our method, it becomes $C=46$. The consequent change in the first-order energy of Li^6 is $-9.1mc^2$ and in $E_D^{(2)}$ is $1.0mc^2$. With the parameters $B=72$, $C=46$, $\alpha=16$, $g=0.205$, the binding energy of Li^6 is then $-E=57.6mc^2$, for the unsymmetrical form. The result is thus quite sensitive to this small readjustment of a parameter to fit the data on the lighter nuclei. This particular readjustment seems to be incompatible with the newest scattering results.[16] Other readjustments are possible. Fitting the He^4 energy by a change of g does not alone have much effect on the Li^6 energy; $(\partial E/\partial g)$ being about $60mc^2$ for He^4 and $70mc^2$ for Li^6. Change of B, α and g simultaneously (approximately scattering requirements) is a possible means of fitting the binding of He^4 (keeping $C=(1-2g)B$ if desired), but it also increases the Li^6 binding not much more than the He^4 binding. Values of the parameters selected to bring about agreement with the binding energies $4.3mc^2$ of H^2, $55mc^2$ of He^4 and $62mc^2$ of Li^6 are $\alpha=16$, $B=72$, $C=47.7$, $g=0.238$, but here C is considerably greater than $(1-2g)B$, which definitely disagrees with the scattering results.[16] This unsymmetrical form of interaction, although comparatively flexible, seems then to be not quite adequate to explain both the binding energies and the scattering data. The binding energy of Li^6 calculated by the symmetrical form (9_s) with our original choice of parameters was in more marked disagreement with experiment than was the result we have just discussed. Furthermore, it is a less flexible form of interaction, containing fewer parameters, and less can be altered in the Li^6 result by adjusting the parameters to fit He^4 by this method: we alter α from 16 to 17, and then change B from 72 to 75.3 to fit the deuteron binding[17] and g from 0.205 to 0.198 to keep the excited level of the deuteron at zero.[18] With the new parameters we find the He^4 energy to be -55.1, while for Li^6 the value of $-E^{(0)}-E^{(1)}$ has been lowered by only $0.3mc^2$ and $-E_D^{(2)}$ by $0.9mc^2$ below the values given in Table V. The final value of the binding energy of Li^6 is thus $45mc^2$. This seems to exclude the interaction used as inadequate (see discussion below).

Other Symmetrical Forms of Interaction

A symmetric form of interaction would add to the elegance of the theory of nuclear binding. Such an interaction is compatible with the scattering results, which seem to require practically equal singlet interactions between like and unlike particles. Although the special and comparatively simple form (9_s) seems to be inadequate, a more general symmetric form may still be successful. The general symmetrical form of interaction

$$U=\sum_{\text{all pairs}} J(r_{ab})O_{ab} \quad \text{with}$$
$$O_{ab}=\{(1-g-g_1-g_\sigma)P_{ab}^{(q)}+gP_{ab}+g_1+g_\sigma P_{ab}^{(\sigma)}\} \tag{17}$$

(where $P_{ab}^{(\sigma)}$ is a permutation operator exchanging spin coordinates only[19]) is equivalent[20] to the forms already used for the two-, three-, and four-body problems if $g+g_\sigma=g_0\approx 0.2$, the constant determined by scattering. We continue to specialize $J(r_{ab})=Be^{-\alpha r^2_{ab}}$. The first-order energy of Li^6 with this form of interaction is

$$E^{(0)}+E^{(1)}=55\alpha\sigma/12-\{5-8g+10g_1 +(8-2g-20g_1-18g_\sigma)/\tau+5/\tau^2\}Bu+0.7(\alpha\sigma)^{\frac{1}{2}}.$$

The matrix elements H_{oa}' calculated by use of this form of U in (3) (neglecting V) have already been listed in Table IV, for the doubly excited states. The contribution of these states to the

[16] Breit, Condon, and Present, reference 2, especially pages 844–45.

[17] Feenberg and Knipp, reference 1, Table III.

[18] As an approximation. Cf. Feenberg and Share, reference 1 Table IV. According to reference 16, the values of g_0 should be larger, thus demanding an increase of B and α, to fit He^4, which does, however, not improve the calculated Li^6 binding appreciably.

[19] J. A. Bartlett, Phys. Rev. **48**, 102 (1936).

[20] Breit and Feenberg, Phys. Rev. **50**, 850 (1936). The equivalence does not extend to our third order.

second-order energy is

$$E_D^{(2)}=-\{52+59g^2+175g_1^2+111g_\sigma^2-62g-50g_1-102g_\sigma-70gg_1+38gg_\sigma+210g_1g_\sigma-(70+10g^2+700g_1^2+394g_\sigma^2+40g-350g_1-240g_\sigma-70gg_1-124gg_\sigma+1050g_1g_\sigma)/\tau+(180+27g^2+700g_1^2+587g_\sigma^2-85g-325g_1-345g_\sigma+140gg_1+86gg_\sigma+1260g_1g_\sigma)/\tau^2-35(2+g+10g_1+9g_\sigma)/\tau^3+214/\tau^4\}\times(Bu/\tau)^2/\alpha\sigma+\{64-126g+270g_1+84g_\sigma+(154-60g-540g_1-480g_\sigma)/\tau+203/\tau^2\}\times(Bu/\tau)/12-(323/288)\alpha\sigma. \quad (18)$$

We wish by use of these expressions to compute the binding energy of Li^6, after determining the parameters, as far as possible, from other considerations. The recent paper on scattering by Breit, Condon and Present[16] indicates that g_0 should exceed (by about 0.04) the value selected to make the excited level of the deuteron zero.[18] This increase of g_0 effects a decrease of the alpha-particle binding, which may be compensated by shortening the range of the interaction and increasing its strength.[8] Parameters thus selected to satisfy the new scattering requirements and to give the observed H^2 and He^4 energies (the latter by this method) are

$$\alpha=22, \qquad g_0=0.22 \qquad B=92. \quad (19)$$

The limits placed on the selection of the g's by Breit and Feenberg's consideration of extreme cases of heavy nuclei[20] may, for our purposes be summarized

$$1.25\geq 1+5g_1+4g_\sigma \quad (20)$$

(which is the second of their Eqs. (7.3), allowing 0.03 for the Coulomb term). It appears from the foregoing that our present task is to try to find values of the parameters which will give a low enough energy for Li^6. Since (20) is a condition that certain extremely heavy nuclei will not have too much binding, we will obtain as much binding as possible by selecting the g's to satisfy (20) as an equality. This limits us to a one-parameter family of choices of the g's, the relations between them being

$$g=0.22-g_\sigma, \qquad g_1=0.25-0.8g_\sigma. \quad (21)$$

Using (19) and (21) we proceed to compute the binding energy of Li^6 for various values of g_σ. The first-order energy is independent of g_σ and has its minimum $E^{(0)}+E^{(1)}=-23.9mc^2$ at $\sigma=1.2$. Introducing (21) in (18) yields

$$E_D^{(2)}=-\{35.8-5.3g_\sigma+20g_\sigma^2-(31.7-19.4g_\sigma+80g_\sigma^2)/\tau+(132.8-17.6g_\sigma+80g_\sigma^2)/\tau^2-166.2/\tau^3+214/\tau^4\}\times(Bu/\tau)^2/\alpha\sigma+\{103.8-6g_\sigma+(5.8+12g_\sigma)/\tau+203/\tau^2\}(Bu/\tau)/12-(323/288)\alpha\sigma. \quad (22)$$

This is evaluated for $\sigma=1.2$ and for several values of g_σ in Table VII. The contribution of the quadruply excited states is more tedious to compute, but was found, using (9_s), to be rather small. We notice that $E_D^{(2)}$ does not differ very much, for rather small values of g_σ, from the value computed using (9_s), and we shall here assume that this is also true of the contribution of the quadruply excited states, and of the other smaller contributions to the energy. We thus subtract about $5mc^2$ from the sum of the values just computed, or about $29mc^2$ from the values of $E_D^{(2)}$ in Table VII, to obtain the energy of Li^6 (experimentally $-62mc^2$) for these parameters. It thus appears to be necessary to go to rather large values of the g's ($g_\sigma\sim\pm 2$ and the others from (21)) in order to find a symmetrical form of interaction, of a single error-curve radial dependence, which satisfies the demands of the scattering data, of the upper limit of nuclear masses, and of the H^2, He^4 and Li^6 energies. It is still possible (but does not seem very likely) that this conclusion would be altered by more complete evaluation of the higher order contributions.

Note added in proof: The g's here required are incompatible with further limitations, implied by an extension of Wigner's considerations of the stability of isobars.* This seems to exclude (17) as inadequate for a *detailed* theory of nuclei. A symmetrical form of interaction with different ranges $\alpha^{-\frac{1}{2}}$ for various P's, or with another radial dependence, is, of course, still a possibility.

Discussion of the Central Approximation

The question arises, whether it would not be better to attack the problem of Li^6 from the other extreme of the binding of a deuteron to an

* Cf. Inglis and Young, Phys. Rev. **51**, 525 (1937). The limitations also remain approximately valid as one departs from the high-density limit.

TABLE VII. $E_D^{(2)}$ *in* mc^2 *for* $\sigma = 1.2$

g_σ	−2	−1	0	1	2
$-E_D^{(2)}$	39.1	24.7	19.7	24.0	37.7

alpha-particle, assuming that they do not distort one another very much. One might expect this approach to be valid if the binding energy of the deuteron to the alpha-particle were much less than the "internal" binding energy of the deuteron itself. In the light of this criterion, let us compare the situation in Li^6 and Li^7. The experimental ratio of the "external" to the "internal" binding energy of the deuteron in Li^6 is approximately $3mc^2/4mc^2$, and the corresponding ratio for the triton in Li^7 is $5mc^2/16mc^2$. It seems from this rough criterion, then, that we are more apt to have a merged nucleus in Li^6 than in Li^7. In Li^7 there are indications[21] that the lowest state is a ^2P, the "orbital" angular momentum being essentially that of one proton. We may conclude that our central approach is probably the more nearly correct in first order.

The problem carried out from that other extreme would presumably yield the lowest energy of the system as a function of a parameter determining the average distance between the particles. The interactions are so chosen as to make this energy approach $-(55+4)mc^2$ asymptotically (from above, the Coulomb range being longest) as the average distance approaches infinity. If, by our central approach, which converges rapidly enough to be practicable only for smaller average distances, we compute with assumed interactions a value of the energy above the asymptotic value, we may conclude that these interactions would not lead to a merged nucleus (if to a stable nucleus at all). The physical argument of the preceding paragraph makes it probable that such interactions are not the correct interactions.

CALCULATION OF THE NUCLEAR MOMENTS

Until now we have assumed that the higher order corrections to the energies of the low configuration do not put some other state below the ^3S. Since the first-order separations of the states are of the order of magnitude $3mc^2$ and the second-order corrections are about $20mc^2$, this is not entirely obvious without further inspection. That the singlets should not descend below the corresponding triplets seems fairly apparent because the interactions have been chosen to make matrix elements smaller between singlets than between triplets, a characteristic which would extend to most of the H_{oa}' also. Of the other two triplets, let us consider for example the ^3D, which is next to the ^3S in first order. A wave function with which we might calculate the energy of the ^3D is $\{(1, 1) - (001, 001)\}/\sqrt{2}$ (an arbitrary choice of one of the degenerate functions allowed by the three-row secular problem above). Using this instead of ψ_0, we would construct a table similar to Table IV. The type of state in Table IV which makes the largest contribution to the second-order energy of the ^3S is (01, 0, 1 : 01, 0, 1) for which $H_{oa}' = (2f_{1100}+2A)/\sqrt{3}$. The corresponding matrix element in the ^3D calculation is $\pm(f_{1100}+A)/\sqrt{2}$ for eight of the states of this type and 0 for the other four. The same tendency for the second-order correction to be largest for the S state appears to pervade the rest of the table. Noting this tendency, we have without further calculation the result that the ^3S, which is the ground state in first order, is the ground state in second order also. This is essentially a calculation of the nuclear angular momentum, $I=1$.

In calculating the higher order corrections to the zero-order[14] magnetic moment, we take $\int \psi^* \Sigma(\xi\partial/\partial\eta - \eta\partial/\partial\xi)\psi d\tau$, summed over protons only, where

$$\psi = \phi_0 + \Sigma\psi_a{}^0 H_{oa}'/(E_0 - E_a) + \Sigma\psi_a\{H_{ab}' - \delta_{ab}\}H_{bo}'/\{(E_0-E_a)(E_0-E_b)\} + \cdots.$$

The first-order correction includes the terms in the first power of H_{oa}', products of the form $H_{oa}' \int \psi_o^*(\xi\partial/\partial\eta - \eta\partial/\partial\xi)\psi_a{}^0 d\tau$. The first factor H_{oa}' has nonvanishing values only for states a with an even sum of the quantum numbers n for each direction. The second factor has nonvanishing values only for states a having Σn_ξ odd and Σn_η odd. All such terms therefore vanish. In considering the second-order correction, the argument must be extended to the case where a nonvanishing term would require a to differ from zero by even Σn_ξ, and b from a by even $\Sigma\Delta n_\xi$, but b from zero by odd Σn_ξ. Thus

[21] D. R. Inglis, Phys. Rev. **50**, 743 (1936).

we see that the higher orders contribute no correction to the orbital part of the magnetic moment. This rule is quite general, for all nuclei, and is of course independent of the error-curve shape of the interaction function here employed. It follows also from conservation of orbital angular momentum, if one thinks of expanding in the ϕ's.

We have therefore to consider only excited states with $M_{S\nu}=3/2$, $M_{S\pi}=-\frac{1}{2}$ or with $M_{S\nu}=-\frac{1}{2}$, $M_{S\pi}=3/2$. The former are exactly as numerous as the latter, in the special case of Li^6, and have exactly corresponding elements H_{oa}', so their contributions to the projected spin magnetic moment, $\int\psi^*(g_\nu\sigma_{z\nu}+g_\pi\sigma_{z\pi})\psi d\tau$, cancel one another. In Li^6 the zero-order result, which makes the magnetic moment of Li^6 equal to that of the deuteron (as observed),[22] is exact (insofar as V is negligible in H_{oa}', cf. reference 14: *note added in proof*).

In other nuclei correction terms appear due to states analogous to the last four types of Table IV. These are small, of order g^2, for the forms of interaction (9), but may be quite large for (17) with large g_σ. There is a remote possibility that they might furnish an additional means of testing the interaction assumptions.

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[22] Manley and Millman, Phys. Rev. **50**, 380 (1936).

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On the Magnetic Scattering of Neutrons

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The scattering of slow neutrons by atoms is considered, assuming that, in addition to the ordinary nuclear forces, there is a magnetic interaction between the neutron and the atomic electrons. It is found that the neutrons scattered from an unpolarized beam will be partially polarized in virtue of this magnetic interaction. Since the scattered intensity depends not only upon the intensity, but also upon the spin density of the incident beam, the polarization thus produced can manifest itself by a second scattering. An expression is derived for the neutron intensity after double scattering from magnetized iron plates. Under optimum conditions, it is found that the scattered intensity with parallel orientation of magnetizations is 15 times that with antiparallel orientation. The partial polarization of the scattered neutrons indicates that the undeviated neutron beam will also have a nonvanishing spin density. Expressions are derived for the intensity and spin density of a neutron beam after traversing a certain thickness of magnetized iron. These results are used in the discussion of three types of experiments for producing and detecting a polarized beam of neutrons.

INTRODUCTION

THE magnetic moment of the neutron has not been measured directly, but has been obtained from the magnetic moments of the proton and the deuteron.[1] The assumption of simple additivity of magnetic moments, involved in this indirect deduction, is, however, open to some objection from the point of view of the β-ray theory of heavy particle interactions and magnetic moments.[2] Since the neutron and proton are symmetrical with respect to interaction with the electron-neutrino field, the magnetic moment of the deuteron should be equal to the "elementary moment" of the proton, $e\hbar/2Mc$. The observed value is $0.85\ e\hbar/2Mc$, which is probably to be explained by the additional moment arising from the process of neutron-proton interaction, and by the fact that the proton is decomposed and does not possess its "elementary moment" during a large fraction of the time.

Recently, Bloch[3] has suggested a direct method of measuring the magnetic moment of the neu-

[1] J. M. B. Kellogg, I. I. Rabi and J. R. Zacharias, Phys. Rev. **50**, 472 (1936).
[2] G. C. Wick, Lincei Rend. **22**, 170 (1935); H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8**, 82 (1936).
[3] F. Bloch, Phys. Rev. **50**, 259 (1936).