Wave Functions for Nuclear Shell Theory by a Variation Method*

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A system of A nucleons with two-nucleon potentials $V(i,k)$ acting between each pair of them is taken as a model for the nucleus. A variation method for obtaining the best approximation to the wave function of this system as a linear combination of a given set of functions, $\psi_1, \cdots, \psi_q$, is presented. In view of the evidence for shell effects, each ψ_α is assumed to describe A identical particles moving in a central field V'. In general, the amplitudes of only a small number of ψ_α are large. For a central Gaussian interaction $V(i,k)$ and a harmonic oscillator potential V', this method can account for the binding energy of one neutron in O^{17}, but not for the total binding energy of O^{16}. The model is compared with a spectroscopic one for a double closed shell core plus outer nucleons.

SUBSTANTIAL experimental evidence has long suggested that single-particle wave functions play a significant role in the description of the state of a nucleus. The earliest and simplest model[1] can be described as follows: The angular momenta of the nucleons of an even-even nucleus couple to total angular momentum $J=0$. A nucleus with odd mass number A consists of an even-even core with $J=0$ and a single outer nucleon, the state of this nucleon being determined by the sequence of levels in an isotropic harmonic oscillator well, assuming strong spin-orbit coupling.

This model can be modified in order to take into account charge-independence of nuclear forces[2,3]: The nucleons are divided into two groups, a core comprised of the number of nucleons needed to form the maximum number of neutron and proton closed shells according to the harmonic oscillator model, and the remaining outer or valence nucleons, which are not sufficient in number to form a closed shell. The outer nucleons are assumed to move in a harmonic oscillator central potential due to the core, and to be subject to an interaction between pairs of nucleons at least resembling that between an isolated system of two nucleons. The possible states of the outer nucleons are determined by the Pauli principle, on the assumption that the states of the core nucleons are already filled. It is evident, however, that if the A nucleons are to be treated as identical particles, they cannot be separated into two groups. The double closed-shell core model therefore fails to take proper account of the total antisymmetry of the nuclear wave function.

1. DESCRIPTION OF THE MODEL

In order to escape this difficulty, let us consider a variation method for solving the total nuclear Hamiltonian of an A-nucleon system under two-nucleon forces:

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \nabla_i^2 + \sum_{i<k=2}^{A} V(i,k). \tag{1}$$

Here ∇_i^2 is the Laplacian operating on the coordinates of the ith particle, m is the mass of the nucleon, and $V(i,k)$ is a potential which may depend upon the spin and isotopic spin components, as well as the coordinates, of particles i and k. Although we would expect $V(i,k)$ to have a central and a tensor term, calculations will here only be made for central forces. The addition of a potential acting upon a single particle, in the form of

$$\sum_{i=1}^{A} W(i), \tag{2}$$

would not alter the main features of this formulation.

In order to solve the equation

$$H\Psi = E\Psi, \tag{3}$$

let us assume that Ψ is a linear combination of q other functions, ψ_α:

$$\Psi(a_1, \cdots, a_q) = \sum_{\alpha=1}^{q} a_\alpha \psi_\alpha. \tag{4}$$

Ψ and the ψ_α are normalized. (When used in the plural sense, ψ_α or a_α will refer to the set of all ψ_α or a_α, with $\alpha=1$ to q.) Further, let us choose the phases so that all a_α are real. In order to minimize the inner product

$$(\Psi, H\Psi) = E(a_1, \cdots, a_q) \tag{5}$$

and still maintain the normalization of Ψ, let us introduce another parameter, λ, in accordance with the method of Lagrangian multipliers. The condition for a stationary point is then:

$$\frac{\partial}{\partial a_\alpha}(\Psi, (H-\lambda)\Psi) = \frac{\partial}{\partial a_\alpha}\left[(\Psi, H\Psi) - \lambda \sum_{\gamma=1}^{q} a_\gamma^2\right] = 0,$$

$$\alpha = 1, \cdots, q. \tag{6}$$

It is convenient to use script letters for the elements of

* Supported by the U. S. Atomic Energy Commission.
[1] M. G. Mayer, Phys. Rev. **78**, 16 (1950); Haxel, Jensen, and Suess, Z. Physik **128**, 295 (1950).
[2] M. H. L. Pryce, Proc. Roy. Soc. (London) **A65**, 773 (1952).
[3] M. G. Redlich, Phys. Rev. **95**, 448 (1954).

the matrix $\|H\|$:

$$\mathcal{3C}_{\alpha\beta}=\|H\|_{\alpha\beta}=(\psi_\alpha,H\psi_\beta). \qquad (7)$$

Since H is Hermitean, Eq. (6) leads to

$$\sum_{\beta=1}^{q} (\mathcal{3C}_{\alpha\beta}-\lambda\delta_{\alpha\beta})a_\beta=0, \quad \alpha=1,\cdots,q. \qquad (8)$$

The solution to this system of q homogeneous equations in q unknowns is obtained by setting the determinant

$$|\mathcal{3C}_{\alpha\beta}-\lambda\delta_{\alpha\beta}|$$

equal to 0. The lowest λ then equals the minimum of the energy (5).

How should the set of trial functions be selected? The qualitative success of the shell model suggests solutions of a Schrödinger equation,

$$H'\psi_\alpha=E'\psi_\alpha, \qquad (9)$$

for A identical particles, each of which moves in the same central field. Then

$$H'=\sum_{i=1}^{A}\left[-\frac{\hbar^2}{2m}\nabla_i{}^2+V'(r_i)\right]. \qquad (10)$$

Since the ψ_α are merely trial functions, it is not necessary to say anything about the origin of this central field. Equation (9) is separable into a sum of single-particle equations, each of which in turn can be separated into radial and angular parts, since V' is a central potential. We assume that ψ_α is an antisymmetrized A-particle wave function. $V(i,k)$ must be invariant under rotations in ordinary space, and will be assumed to be invariant under rotations in isotopic spin space. Ψ then has definite isotopic and ordinary spin, (T,J), and the same may be assumed for the ψ_α. It should be noted that for a complete set of antisymmetric ψ_α, diagonalization of the matrix $\|H\|$ (with $q=\infty$), would lead to an exact expansion of Ψ. The variation process merely leads to the best approximation in terms of a set of q definite ψ_α. The kinetic energy part, $\mathcal{3C}$, of a matrix element of $\mathcal{3C}$ equals that for $\mathcal{3C}'$, the corresponding matrix for (10):

$$\mathcal{3C}_{\alpha\beta}=-\frac{\hbar^2}{2m}\sum_{i=1}^{A}(\psi_\alpha,\nabla_i{}^2\psi_\beta)=\mathcal{3C}_{\alpha\beta}'. \qquad (11)$$

The potential energy part of a matrix element is

$$\mathcal{V}_{\alpha\beta}=\sum_{i<k=2}^{A}(\psi_\alpha,V(i,k)\psi_\beta). \qquad (12)$$

This is by no means the same for $\mathcal{3C}$ and $\mathcal{3C}'$. It can be separated into a sum of three terms: (a) Terms involving only states belonging to closed shells; (b) terms between an outer state (of an unfilled shell) and all closed shells; (c) terms between outer states only. The phrase "interaction between *states*" instead of *nucleons* is used

here, since it is not possible to associate a nucleon with a definite state.

2. ASSUMPTIONS FOR $V(i,j)$ AND $V'(r_i)$

In the next section, some calculations for the oxygen region will be made. A central Gaussian two-nucleon interaction which leads to the binding energy of the deuteron and to the effective range and scattering length for low-energy neutron-proton scattering in the triplet state will be assumed:

$$V_X(i,j)=V_X(r_{ij})=-V_0P_X\exp(-r_{ij}{}^2/2.245). \qquad (13)$$

Here $P_W=1$, $P_M=$ space-exchange operator, $P_B=$ spin-exchange operator, and $P_H=P_MP_B$. The internucleon coordinate r_{ij} and all other radial coordinates and radii are in units of 10^{-13} cm. The depth $V_0=70.8$ Mev leads to the deuteron binding energy and will be used here.

For $V'(r_i)$ we shall assume a harmonic oscillator potential,

$$V'(r_i)=(\hbar\nu r_i)^2/2m, \qquad (14)$$

with ν determined from

$$\int_0^\infty R_{nl}(r_i)^2r_i{}^2dr_i=(2n+l-\tfrac{1}{2})\nu^{-1}=\mathcal{R}_m(nl)^2. \qquad (15)$$

Here $R_{nl}(r_i)/r_i$ is the radial wave function of particle i moving in potential (14), and n denotes the number of nodes of R_{nl} and l the orbital angular momentum. $\mathcal{R}_m(nl)$ is a quantity about equal to the nuclear radius. We shall make calculations with several values ν_a of ν which are given, together with $\mathcal{R}_m$, in the following table:

a	0	1	2	3	
ν_a	0.250	0.356	0.462	0.568	$\times 10^{26}$ cm^{-2}
$\mathcal{R}_m(1d)$	3.74	3.14	2.76	2.48	$\times 10^{-13}$ cm
$\mathcal{R}_m(1p)$	3.16	2.65	2.33	2.10	$\times 10^{-13}$ cm

In Fig. 1,

$$P_{nl}(r_1)=R_{nl}(r_1)^2 \qquad (16)$$

is plotted against r_1 for $nl=1d$ and $2s$, and parameter ν_1. Here $P_{nl}(r_1)\delta r_1$ is the probability that a particle of type nl be found at some point of an interval δr_1 with r_1 at its center. For reference, the quantity $1.4\times 17^{\frac{1}{3}}=3.60$, the radius of O^{17}, is given on the abscissa. A $1d$ particle will be found at $r_1<3.60$ about 76 percent of the time. This value of ν, or even a somewhat larger one, therefore seems a reasonable choice. The same potential, (14), will be used for all single-particle functions. However, the possibility of using different potentials for different shells has been pointed out.[4] The potentials (13) and (14) with ν_0 were used in reference 2.

It may be worth while at this point to use the potential (14) and the harmonic oscillator wave func-

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[4] E. H. Kronheimer, Phys. Rev. **96**, 1680 (1954).

tions with parameter ν to illustrate the present method. Let us consider a single particle with radial coordinate r moving in another harmonic oscillator potential, $(\hbar\omega r)^2/2m$. This potential will now be substituted for the one in (1) and the variation method with just the ψ_α obtained from (10) with $A=1$ and the potential (14) will be applied. If all R_{nl} are taken as the set of ψ_α, then the a_n are given by the expansion (α now is just ns):

$$\Psi(r)=R_{1s}{}^{(\omega)}(r)=\sum_{n=1}^{\infty} a_n R_{ns}{}^{(\nu)}(r). \tag{17}$$

The first three a_n are:

$$a_1=\left(\frac{2(\nu\omega)^{\frac{1}{2}}}{\omega+\nu}\right)^{\frac{3}{2}}; \quad a_2=\left(\frac{3}{2}\right)^{\frac{1}{2}}\left(\frac{\omega-\nu}{\omega+\nu}\right)a_1;$$
$$a_3=\left(\frac{15}{8}\right)^{\frac{1}{2}}\left(\frac{\omega-\nu}{\omega+\nu}\right)^2 a_1. \tag{18}$$

If we had happened to choose ν equal to ω, the series would have had exactly one term. For $\nu=1.2\omega$, $a_1=0.993$, $a_2=-0.110$, and $a_3=0.011$. The larger $\omega-\nu$ is, the larger is the number of terms necessary to obtain a good approximation to Ψ. In general, the most felicitous choice of ν leads to a minimum of configuration interaction. In this example, it leads to minimal (namely 0) admixtures of the configurations $(2s)^1$, $(3s)^1$, etc., to the $(1s)^1$ configuration.

3. CALCULATIONS ON THIS MODEL

The matrix elements of $\mathcal{3C}$ can be obtained by methods known from atomic spectroscopy. It is convenient to calculate in an

$$nlm_l s m_s l \mu_t \tag{19}$$

representation. Here, the state of each nucleon is specified by one set of quantum numbers (19). t is isotopic spin and equals $\frac{1}{2}$; μ_t is its ζ component. The matrix elements of the kinetic energy are readily calculated, since it is a single-particle operator. It is convenient to introduce some detailed notation for the terms of type (a) and (b) (see Sec. 1) of a diagonal matrix element of the potential energy, on the assumption of central two-nucleon forces. The interaction between one outer $n'l'$ state and all the states of the nl double closed shell will be denoted

$$\mathcal{U}_X(n'l',nl^{8l+4}), \tag{20}$$

where X indicates the type of exchange force, as in Eq. (13). The interaction of a double closed nl^{8l+4} shell with itself will be denoted

$$\mathcal{U}_X(\mathbf{nl}^{8l+4}), \tag{21}$$

with boldface $\mathbf{nl}^{8l+4}$. The quantities (20) and (21) are given in terms of radial integrals by formulas $9^6(11)$
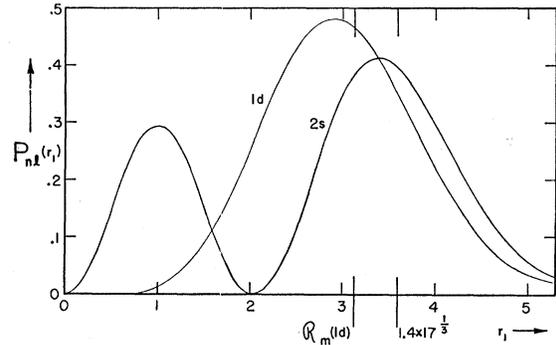

FIG. 1. The probability per unit radial distance, $P_{nl}(r_1)$, that an nl particle be found at r_1, for $nl=1d$ and $2s$. The well parameter is ν_1. The coordinate r_1 is given in 10^{-13} cm.

and $9^6(12)$ of Condon and Shortley,[5] with an obvious modification to take into account isotopic spin and exchange forces. The interaction (21) may be expressed in terms of (20) as follows:

$$\mathcal{U}_X(\mathbf{nl}^{8l+4})=2(2l+1)\cdot \mathcal{U}_X(nl,nl^{8l+4}). \tag{22}$$

The radial integrals for the potentials of the preceding section will be calculated by the method of Talmi.[6] It is important to note that (20) is independent of m_l', m_s', and μ_t'. The terms of type (c) can be obtained from an antisymmetric wave function of the outer nucleons only. [This is plain from reference 5, $7^6(7)$.]

For double closed $1s$ and $1p$ shells the following abbreviation is convenient:

$$(\text{c.s.})=1s^4 1p^{12}. \tag{23}$$

Then one can write

$$\mathcal{U}_X(n'l',\text{c.s.})=\mathcal{U}_X(n'l',1p^{12})+\mathcal{U}_X(n'l',1s^4). \tag{24}$$

The total interaction for (c.s.) is

$$\mathcal{U}_X(\mathbf{c.s.})=\mathcal{U}_X(\mathbf{1s}^4)+\mathcal{U}_X(\mathbf{1p}^{12})+4\mathcal{U}_X(1s,1p^{12}). \tag{25}$$

The Wave Function of O^{17}

The a_α in an expansion (4) for the wave function of a system of 17 nucleons with two-nucleon potential

$$V(i,j)=\frac{1}{2}[V_W(i,j)+V_M(i,j)] \tag{26}$$

will now be estimated, on the assumption of (14) with parameter ν_1. Let us set $q=3$ and denote by ψ_0, ψ_1, and ψ_2 the wave functions for the configurations $(\text{c.s.})(1d)^1$, $(\text{c.s.})(2d)^1$, and $(\text{c.s.})(1p)^{-2}(1d)^3$, respectively. We obtain the following 3×3 matrix for $\mathcal{3C}$, with rows and columns labeled by $\alpha=0$, 1, and 2:

$$\begin{array}{c c c c} & 0 & 1 & 2 \\ 0 & \mathcal{3C}_{00} & -5.0 & (-7.3) \\ 1 & -5.0 & \mathcal{3C}_{00}+26.4 & 0 \\ 2 & (-7.3) & 0 & (\mathcal{3C}_{00}+31) \end{array}. \tag{27}$$

[5] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, London, 1951), second edition.
[6] I. Talmi, Helv. Phys. Acta **25**, 185 (1952).

TABLE I. In this table the following calculated quantities are given in Mev for two values of the well parameter ν: (1) The interaction $\mathcal{V}_X$ between one nl state and all the states of the double closed $1s$ and $1p$ shells. $\mathcal{V}_H$ is given by Eq. (30). (2) The kinetic energy $\mathcal{K}_1(nl)$ for the nl state. (3) The calculated binding energy $\mathcal{B}_1(nl; x)$ of one neutron in O^{17}, defined by Eq. (31).

Calculated quantity	$\nu = \nu_0$	ν_1
$\mathcal{V}_W(1d,\text{c.s.})$	-36.2	-59.5
$\mathcal{V}_M(1d,\text{c.s.})$	-11.2	-11.6
$\mathcal{V}_B(1d,\text{c.s.})$	-10.0	-19.1
$\mathcal{V}_W(2s,\text{c.s.})$	-45.2	-73.0
$\mathcal{V}_M(2s,\text{c.s.})$	-7.2	-4.2
$\mathcal{V}_B(2s,\text{c.s.})$	-15.2	-27.5
$\mathcal{K}_1(1d) = \mathcal{K}_1(2s)$	18.0	25.6
$\mathcal{B}_1(1d; 0.5)$	5.7	10.0
$\mathcal{B}_1(2s; 0.5)$	8.2	13.0
$\mathcal{B}_1(1d; 0.4)$	3.2	5.2
$\mathcal{B}_1(2s; 0.4)$	4.4	6.1

The elements are in Mev; those not enclosed in parentheses have been calculated directly. The cross term $\mathcal{K}_{02}$ was estimated as

$$\mathcal{K}_{02} = \mathcal{K}_{20} \sim \langle 1p^2, L=0 \,|\, V(1,2) \,|\, 1d^2, L=0 \rangle$$
$$= -7.3 \text{ Mev}, \quad (28)$$

since ψ_0 and ψ_2 differ by two single-particle states. An exact calculation, in terms of fractional parentage coefficients, would lead to a sum of several terms like (28) with different L, and probably to a smaller magnitude of $\mathcal{K}_{02}$. There is no kinetic energy contribution, because the angular parts of the single-particle wave functions are orthogonal.

The difference in potential energy between $\mathcal{K}_{22}$ and $\mathcal{K}_{00}$ was estimated as a sum of these terms: (1) The interaction between two $1d$ states and (c.s.). This is a lower limit to the actual contribution, since only 14, instead of 16 particles remain in $1p$ and $1s$ states. (2) The energy of the configuration $(1d)^3$ estimated as that for the lowest state of $(1d_{5/2})^3$. (3) The difference in total potential energy between configurations $(1p)^{10}$ in the $L=0$ state, which is lowest, and $(1p)^{12}$. (4) The interaction between two $1p$ states and $(1s)^4$ must be subtracted. In its place, the interaction between two $1d$ states and $(1s)^4$ is included in term (1).

From the matrix (27) and perturbation theory,

$$a_1 \approx -0.19, \quad a_1^2 \approx 0.036, \quad (29)$$

and $a_2 \approx -0.24$. It should be recalled, however, that the estimates of $\mathcal{K}_{02}$ and $\mathcal{K}_{22}$ are expected to be larger and smaller, respectively, than their actual values. An accurate calculation, therefore, is expected to lead to a smaller absolute value of a_2. A more accurate wave function would be obtained by taking a larger set of ψ_α. These would involve further breaking up of (c.s.) or nd states with $n > 2$. The energies of these states will be considerably higher than those of ψ_0 and ψ_1. Furthermore, the off-diagonal terms $\mathcal{K}_{0\alpha}$ involving them will generally be smaller than $\mathcal{K}_{01}$. Their amplitudes a_α will therefore be smaller than a_1.

The Neutron Binding Energy of O^{17}

ψ_0 alone will be used for this calculation, and a similar wave function, for the configuration (c.s.), for O^{16}. The difference in potential energy between the two nuclei is merely one term of type (b), given by (24). The results are presented in Table I for three types of forces; for the fourth, they can be obtained from

$$\mathcal{V}_H(nl,\text{c.s.}) = -\mathcal{V}_B(nl,\text{c.s.}). \quad (30)$$

Two parameters, ν_0 and ν_1, were used. $\mathcal{K}_1(nl)$ is the kinetic energy of a single nl state. The neutron binding energy is defined as

$$\mathcal{B}_1(nl; x) = -x\mathcal{V}_W(nl,\text{c.s.})$$
$$- (1-x)\mathcal{V}_M(nl,\text{c.s.}) - \mathcal{K}_1(nl). \quad (31)$$

It is also given in Table I, and found to be generally of the order of magnitude of the experimental[7] value of 4.14 Mev, for $x=0.4$ to 0.5. We cannot expect accurate agreement with experiment for two reasons: (1) $\mathcal{B}_1$ is the difference between two large quantities, neither of which can be expected to be very accurate in this approximation. (2) The present model does not account for the difference between the $5/2+$ and $3/2+$ states of O^{17}. We recall that the quantity $\mathcal{V}_X(1d,\text{c.s.})$ is independent of the orientation of the spin and angular momentum of the $1d$ particle. The model does yield a difference between $\mathcal{B}_1(1d; x)$ and $\mathcal{B}_1(2s; x)$.

The Binding Energy of O^{16}

We again assume the pure configuration (c.s.) for O^{16}. The admixtures of higher configurations can be expected to be no larger than the ones found for O^{17}. The total potential energy,

$$\mathcal{V}_X = \mathcal{V}_X(\text{c.s.}), \quad (32)$$

then consists just of type (a) terms. It is given in Table II for various values of ν. The total kinetic energy $\mathcal{K}$ is also given. The Coulomb energy can be calculated from the usual formula as $\mathcal{C} = 14$ Mev. The total binding energy is defined as

$$\mathcal{B}(x) = -x\mathcal{V}_W - (1-x)\mathcal{V}_M - \mathcal{K} - \mathcal{C}, \quad (33)$$

and given in Table II for $x=0.5$ and 0.1. The experimental value[7] is $127.6 = 7.98 \times 16$ Mev.

The table reflects a very large increase of $-\mathcal{V}_W$ with ν, i.e., with decreasing radius. This is a well-known effect. There is an increase of $-\mathcal{V}_M$ with ν also, but it is less rapid than that of $\mathcal{K}$, which is proportional to ν. The quantity $-\mathcal{V}_B$ increases with ν at a rate which lies between that of $-\mathcal{V}_W$ and $\mathcal{K}$.

In making this calculation for the configuration (c.s.) alone, we have, in effect, already applied the present variation method in an approximate way, since it was plain for parameter ν_1, at least, that the minimum

[7] F. Ajzenberg and T. Lauritsen, Revs. Modern Phys. 27, 77 (1955).

energy will appear for a wave function with only small admixtures of wave functions of other configurations. In Table II, the effect of these small admixtures upon the binding energy has been neglected, not only for ν_1, but for the other values of ν as well. Actually, the example at the end of Sec. 2 showed that a change in ν corresponds to a change in the amplitudes of the various states. If, however, these changes are not substantial, which seems likely, then we are justified in considering, as an approximation, only the configuration (c.s.). If the model is correct, we would then expect to obtain a minimum in the energy of the system for a value of ν about equal to ν_1, which corresponds to the radius of O^{16} deduced from experiment. Furthermore, the magnitude of the energy at this minimum should equal the experimental binding energy. An examination of Table II indicates that for a combination of ordinary (W) and space-exchange (M) forces, a minimum does appear at ν_1 for $-\mathscr{B}(0.1)$. The magnitude of $\mathscr{B}(0.1)$, however, is too small by about a factor of 2. For an intermediate value of x, like 0.2, $\mathscr{B}(x)$ will have a maximum value equal to the experimental binding energy; but this appears at about ν_3, which leads to far too small a radius. The binding energy of one neutron in O^{17} would be negative with such a low x, even at ν_3. Furthermore agreement between theory and some experimental quantities for $A=18$ and 19 can be obtained[8] with ν_1, but not with ν_3. It does not appear that spin-exchange (B) or space-and-spin-exchange (H) forces could improve this situation substantially. Thus we see that while the present model with central $V(i,j)$ can account for the binding energy of a neutron in O^{17}, it cannot account for the total binding energy of O^{16}, nor, consequently, for the total binding energy of O^{17}.

4. COMPARISON OF THE VARIATION METHOD WITH WITH THE DOUBLE CLOSED SHELL CORE MODEL

(1) The present formulation will be compared with a model which assumes that B identical outer nucleons move in the field of a double closed shell core. To be specific, let us consider a nucleus with

$$A = 16 + B$$

particles, and a (c.s.) core. We compare the expansion of Ψ given by (4) with

$$\Phi(b_1, \cdots, b_P) = \sum_{\alpha'=1}^{p} b_{\alpha'} \varphi_{\alpha'}, \qquad (4')$$

where the $\varphi_{\alpha'}$ are antisymmetric wave functions for B particles, whose states in $V'(r_i)$ are neither $1s$ nor $1p$. To each $\varphi_{\alpha'}$ there corresponds a ψ_α, which is antisymmetric in A particles and includes the 16 states of (c.s.). The converse is not true, since among the ψ_α there may be some for configurations which do not include (c.s.). The considerations of the preceding

[8] M. G. Redlich, following paper [Phys. Rev. 99, 1427 (1955)].

TABLE II. The following quantities have been calculated for a system of 16 identical particles occupying all the states of the $1s$ and $1p$ double closed shells: (1) The total potential energy, $\mathcal{U}_X$, for four types of interaction. (2) The total kinetic energy $\mathcal{K}$. (3) The total binding energy $\mathscr{B}(x)$, defined by Eq. (33). Results are given here in Mev for several values of ν, defined in Sec. 2.

Calculated quantity	$\nu = \nu_0$	ν_1	ν_2	ν_3
$\mathcal{U}_W$	−428	−680	−939	−1201
$\mathcal{U}_M$	−236	−310	−360	−396
$\mathcal{U}_B = -\mathcal{U}_H$	−77	−148	−232	−322
$\mathcal{K}$	185	263	341	419
$\mathscr{B}(0.5)$	133	218	294	366
$\mathscr{B}(0.1)$	56	70	63	43

section for the wave function of O^{17}, however, indicate that the amplitudes of such ψ_α are small. If we neglect them, and consider

$$\Psi' = \sum_{\alpha=1}^{p} a_\alpha \psi_\alpha, \qquad (4'')$$

where the sum extends only over those ψ_α whose configurations include (c.s.), then a correspondence between Ψ' and Φ may be established.

Let us consider first two Hamiltonians, H, defined by (1), and

$$G = -\frac{\hbar^2}{2m} \sum_{i=17}^{A} \nabla_i^2 + \sum_{i>k=17}^{A} V(i,k). \qquad (1')$$

Their matrices are $\mathcal{K}$, given by (7), and $\mathcal{G}$ given by

$$\mathcal{G}_{\alpha'\beta'} = \|G\|_{\alpha'\beta'} = (\varphi_{\alpha'}, G\varphi_{\beta'}). \qquad (7')$$

We shall assume in the following argument that the outer particles are only in $1d$ and $2s$ states. In general, higher states [for potential (14), states of higher harmonic oscillator shells] will be present, but with much smaller a_α. It appears, however, that coefficients of states of several configurations of type

$$(1d)^k (2s)^{B-k}, \qquad (34)$$

are sometimes large.[3,8,9] States may be described as follows:

$$\alpha = \text{(c.s.)}(1d)^{k(\alpha)} (2s)^{B-k(\alpha)} K, T, J; \quad \alpha' = \text{(c.s.)}^{-1}\alpha. \qquad (35)$$

K stands for all other quantities necessary to describe the state, e.g., intermediate angular momenta.

It is plain that

$$\mathcal{K}_{\alpha\alpha} = \mathcal{G}_{\alpha'\alpha'} + E(\text{c.s.}) + k \cdot E(1d) + (B-k) \cdot E(2s), \qquad (36)$$

where $E(\text{c.s.})$ is the total energy of (c.s.) and

$$E(nl) = \mathcal{K}_1(nl) + \mathcal{U}(nl, \text{c.s.}). \qquad (37)$$

$\mathcal{U}$ stands for any combination of the $\mathcal{U}_X$. In actually making calculations it is desirable to introduce

$$C(2s, 1d) = E(2s) - E(1d). \qquad (38)$$

[9] J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) A229, 536 (1955).

C is a theoretical quantity, which can be obtained from Table I of the last section. [If a simple spin-orbit operator of type

$$-2.03 \sum_{i=17}^{A} \mathbf{l}_i \cdot \mathbf{s}_i \text{ Mev} \tag{39}$$

is also introduced,[9] then it is possible to account by (38) with an empirical $C = -1.15$ Mev and (39) for the energy differences between the three lowest states with positive parity of O^{17}.]

A calculation similar to that for $\mathcal{U}_X(n'l', nl^{8l+4})$ shows that for central forces an interconfiguration matrix element of type (b) vanishes, unless the two configurations differ only in the radial quantum number n of one single-particle state. If, further, states of the same configuration which differ only in K are orthogonal, then the total type (b) matrix element between them is also 0, as may be seen from expansions of the ψ_α in fractional parentage coefficients. It follows for states of the configurations (34) that

$$\mathcal{3C}_{\alpha\beta} = \mathcal{G}_{\alpha'\beta'}, \ \alpha \neq \beta. \tag{40}$$

Diagonal elements of $\mathcal{3C}$ and $\mathcal{G}$ thus differ only by

$$E(\text{c.s.}) + B \cdot E(1d), \tag{41}$$

which is constant for all of them, and

$$[B - k(\alpha)] \cdot C(2s, 1d), \tag{42}$$

which is not. The off-diagonal elements are the same. It is plain that solution of the secular equation of a new matrix whose elements are

$$\mathcal{G}_{\alpha'\beta'}' = \mathcal{G}_{\alpha'\beta'} + [B - k(\alpha)] \cdot C(2s, 1d) \cdot \delta_{\alpha\beta} \tag{43}$$

leads to a Φ with amplitudes $b_{\alpha'}$ equal to the corresponding ones of Ψ'. That is,

$$b_{\alpha'} = a_\alpha.$$

It must be emphasized that this equivalence is essentially a formal one, brought about by the theoretical possibility for inclusion of the differences in type (b) terms in a simple way.

The physical difference between the two models is very obvious. The double closed shell core formulation does not automatically ensure that there will be no overlapping of the space wave functions of outer and inner (core) nucleons which have the same spin and isotopic spin components. For harmonic oscillator wave functions such overlapping is not small. This is evident from an examination of the direct and exchange contributions to $\mathcal{U}_X(1d,\text{c.s.})$. These follow, for parameter ν_1:

	Direct term	Exchange term	Total
$\mathcal{U}_W(1d,\text{c.s.})$	-66.5	7.0	-59.5 Mev
$\mathcal{U}_M(1d,\text{c.s.})$	-28.2	16.6	-11.6 Mev

The exchange terms are seen to contribute -11.8 Mev to the binding energy of one neutron, $\mathcal{B}_1(1d; 0.5)$, in O^{17}. In other words, the double closed shell core formulation is exact only if an impenetrable wall encloses the core.

(2) The operators for most observable quantities can be expressed as nonscalar single-particle irreducible tensor operators $T^{(k\kappa)}$ of order k in ordinary and κ in isotopic spin space, or as sums of such operators. It can be shown that matrix elements of such operators are the same for Ψ' and Φ. Let us define

$$T_{(N)} = \sum_{i=1}^{N} T^{(k\kappa)}(i), \tag{44}$$

where $T^{(k\kappa)}(i)$ operates on the space, spin, and isotopic spin co-ordinates of particle i. At least one of k and κ is $\neq 0$. It is convenient to consider again the representation

$$\alpha = a_1, \cdots, a_A \ \text{with} \ a_i = l_i m_{li} s_i m_{si} t_i \mu_{ti}. \tag{45}$$

Also

$$(\text{c.s.}) = a_1, \cdots, a_{16} \ \text{and} \ \alpha' = a_{17}, \cdots, a_A. \tag{46}$$

The diagonal matrix element of $T_{(A)}$ is just

$$\langle \alpha | T_{(A)} | \alpha \rangle = \sum_{i=1}^{A} \langle a_i | T^{(k\kappa)} | a_i \rangle, \tag{47}$$

from $6^6(9)$ of Condon and Shortley.[5] Then

$$\langle \alpha | T_{(A)} | \alpha \rangle = \langle \text{c.s.} | T_{(16)} | \text{c.s.} \rangle + \langle \alpha' | T_{(B)} | \alpha' \rangle. \tag{48}$$

Equation (47) shows that the first term of (48) is exactly the diagonal matrix element for the one state of (c.s.). That state belongs to representations of order 0 in both ordinary and isotopic spin space. The same is not true of $T_{(16)}$, so that its matrix element is 0 by the vector addition rule. The second term of (48) is the diagonal matrix element for Φ. Only the second term of (48) appears in off-diagonal matrix elements; thus the entire matrix of $T_{(A)}$ equals that of $T_{(B)}$.

Formula (47) reminds us that center of mass effects are not accounted for in the variation formulation. (47) leads to zero quadrupole moment for O^{17} if ψ_0 of Sec. 3 is assumed, contrary to experiment. If the double closed shell core model is used, on the other hand, O^{17} consists of a core and one outer nucleon, and it is easy to calculate the effect of the core upon the quadrupole moment.

Calculations using $V(i,j)$ and $V'(r_i)$ of Sec. 2 for the double closed shell core model modified by the terms (39) and (42) have been made in reference 3 for $B = 2$ and in the following paper for $B = 3$.