Self-Consistent Treatment of the Independent-Particle Central-Field Nuclear Model

G. E. TAUBER, *Department of Physics, Western Reserve University, Cleveland, Ohio*

AND

TA-YOU WU, *Division of Pure Physics, National Research Council, Ottawa, Canada*

(Received May 4, 1956)

The purpose of the present work is, starting from a given assumed nucleon-nucleon interaction $V(\mathbf{r}_i-\mathbf{r}_j)$ and the independent-particle, central-field approximation, to deduce all the consequences of this model by means of the Hartree-Fock-Slater theory. The $V(\mathbf{r}_i-\mathbf{r}_j)$ is chosen to satisfy the saturation requirement and to be consistent with some of the properties of the two-nucleon system, but contains the strength factor V_0 as an undetermined parameter. This V_0 and the single-particle wave functions $\psi_n(\mathbf{r}_i)$ are determined by the variational principle together with the requirement that the total binding energy of the nucleus be equal to its empirical value. The binding energies of the individual nucleons in the various shells are themselves approximately given by the Fock equations which also lead to a central field which is different for the different shells. The average central field implied in the usual treatment of the shell model is, however, the same for a nucleon in any shell, and this must be identified with some approximate average field obtained by a procedure such as that suggested by Slater for an electron in an atom or in a metal. On the other hand, the central field in the sense of Hartree (i.e., obtained from the Fock theory by neglecting the exchange terms) would be a very poor approximation as the exchange terms are not negligible compared with the direct terms. It is emphasized in the present work that the application of the variational principle to the problem rids the shell model of the inconsistent procedure in the usual treatments in which two independent assumptions concerning $V(\mathbf{r}_i-\mathbf{r}_j)$ and the average central field $V(\mathbf{r})$ are made. A comparison of the result of the present program with the empirical facts will form a correct basis on which to judge the fairness or failure of the central-field approximation in the shell model.

Numerical calculations have been carried out for the O^{16}, O^{15}, and O^{17} nuclei to illustrate the ideas of the self-consistent treatment of the independent-particle, central-field nuclear model. In a first approximation, the V_0 and the wave functions $\psi_n(\mathbf{r}_i)$ are determined by the modified Ritz method. The binding energies and the effective "central fields" for the individual nucleons in the various shells are then calculated from the Fock equations by means of these $\psi_n(\mathbf{r}_i)$. It is found that the parameter V_0 in O^{16}, O^{17}, and O^{15} comes out to be very nearly the same, that the Fock central potentials are considerably lower than the Hartree potentials; that the former exhibit a general shape of a wine-bottle with a diffuse boundary; and that the "binding energy of the last nucleon" does not come out very well from the Fock equations.

I. INTRODUCTION AND AN OUTLINE OF THE PRESENT WORK

IN the well-known nuclear shell model of Mayer, Jensen, *et al.*,[1] each nucleon is assumed to move in a central field $V(r)$ arising from the interaction between that nucleon and the other nucleons in the nucleus. The assumption of a reasonable potential $V(r)$ together with a strong interaction between the spin and the orbit of each nucleon determines the energy levels of each nucleon. This model finds an immediate success in accounting for the so-called magic-number nuclei, the spins and the magnetic moments of many nuclei. When attempts are made to calculate such properties as the energies, spins, parities and magnetic moments of the excited states of a nucleus on this model, it has been customary in the literature to assume a certain central field $V(r)$ for the interaction of each individual nucleon with all the other nucleons in the nucleus, and an interaction $V(\mathbf{r}_i-\mathbf{r}_j)$ between any two nucleons that lie outside a closed shell and whose configurations are being calculated. A knowledge of $V(r)$ is necessary in order to obtain the individual-nucleon wave functions in terms of which the properties of the nucleus arising from the nucleons outside the closed shells are calculated. In most of the existing work on the basis of this shell model, various specific forms have been assumed for $V(r)$ and $V(\mathbf{r}_i-\mathbf{r}_j)$.[2] Certain successes in accounting for certain observed energy levels, their spin and parities, etc., have been achieved by properly choosing these potentials, together with some further refinements in the original model so as to include the effect of intermediate couplings and the deviations of $V(r)$ from a spherically symmetric field. But despite these successes, a feature remains in these studies that seems unsatisfactory, namely, separate assumptions seem to have been made for the central field $V(r)$ and the pair-interaction $V(\mathbf{r}_i-\mathbf{r}_j)$.[3] These two potentials are not independent, but are connected by simple, definite relations from the point of view of the self-consistent field method of Hartree-Fock-Slater.

The purpose of the present work is to carry out a self-consistent treatment of the central-field nuclear shell model. One starts with a pair interaction $V(\mathbf{r}_i-\mathbf{r}_j)$ for two nucleons inside a nucleus which satisfies the requirement of saturation of nucleus forces and is chosen to be consistent with some of the properties for a pair of "free" nucleons (i.e., not inside a nucleus). This potential $V(\mathbf{r}_i-\mathbf{r}_j)$ is to contain an adjustable parameter which, together with the single-nucleon wave functions $\psi_n(\mathbf{r}_i)$, is to be determined by means of the variational principle and the empirical value of the total binding energy of the nucleus (Secs. II, III). No independent assumption about a central field $V(r)$

[1] M. G. Mayer, Phys. Rev. **78**, 16 (1950); Haxel, Jensen, and Suess, Phys. Rev. **75**, 1766 (1949).

[2] A. M. Lane, Proc. Phys. Soc. (London) **A68**, 197 (1955), and references given there.

[3] For example, M. G. Redlich, Phys. Rev. **99**, 1421 (1955).

will be made so that there is no internal inconsistency in the theory.

This determination of $V(\mathbf{r}_i-\mathbf{r}_j)$ would by itself not be of any particular interest since it is the immediate result of our assumptions, namely, the "central field" approximation and the various properties imposed on $V(\mathbf{r}_i-\mathbf{r}_j)$. For this "central field" approximation to form a useful basis for a nuclear model, it is necessary that the closed-shell structures do stand out from the neighboring nuclei in having greater stabilities. This is not at all obvious as in the case of the electronic structure in the atoms. The nuclei differ from the atoms in two fundamental aspects, namely (i) the absence of a predominating attractive central Coulomb field and (ii) the saturation property of the nucleon interaction $V(\mathbf{r}_i-\mathbf{r}_j)$. In the case of the atoms of nuclear charge Ze, it is a good qualitative approximation to regard each electron as moving in a central field $V(r)$ (for example, a Thomas-Fermi field) which behaves as

$$\lim_{r\to 0} rV(r)\to Ze, \quad \lim_{r\to\infty} rV(r)\to e.$$

In the case of the nuclei, the central field approximation itself is no longer such a natural one, but has assumed the nature of a strong assumption.[4] It is therefore necessary to examine the consequences of the central-field approximation by means of the Hartree-Fock-Slater method which gives the most general theory consistent with the central-field approximation.

For this purpose, we give in Sec. V the Hartree-Fock equations for the various "orbitals" in the O^{15}, O^{16}, and O^{17} nuclei. The $V(\mathbf{r}_i-\mathbf{r}_j)$ for O^{16} is determined in Secs. II and III. One may make the assumption that for neighboring nuclei such as O^{15}, O^{16}, O^{17} the pair-interaction $V(\mathbf{r}_i-\mathbf{r}_j)$ is the same. With this $V(\mathbf{r}_i-\mathbf{r}_j)$ from O^{16}, one can obtain the (approximate) binding energies of the individual nucleons in the various shells in these nuclei from the eigenvalues of the Hartree-Fock equations (Sec. VI), or one can calculate the total binding energy of O^{15} (Sec. IV) by means of the method of Secs. II and III, with the $V(\mathbf{r}_i-\mathbf{r}_j)$ as determined from O^{16}. Or one may reverse the procedure by carrying out similar but independent variational calculations (as in Secs. II and III) for O^{15}, O^{16}, and O^{17} and see if the $V(\mathbf{r}_i-\mathbf{r}_j)$ so determined for the different nuclei are reasonably close to one another. In Sec. VI, the "central fields" for the individual nucleons are given for both the Fock and the Hartree theory and the difference between them emphasized.

The treatment illustrated by the O^{15}, O^{16}, and O^{17} nuclei in the present work can obviously be extended to any nuclei. To explore and exhaust the possibilities and limitations of the individual-particle model as contrasted with the "collective model," the present writers plan to further refine and extend the treatment here by introducing nucleon-nucleon correlations in the wave functions so as to include the polarization effect, by introducing spin-orbit or tensor forces, and to treat such problems as the distribution of the neutrons and the protons in the heavy nuclei. Work on this program is being carried out and will be reported in due course.

II. VARIATIONAL TREATMENT OF A NUCLEUS IN THE INDEPENDENT-PARTIAL MODEL

Let the Hamiltonian of a nucleus be

$$H=\sum_i H(i)+\sum_{i\neq j} V(\mathbf{r}_i-\mathbf{r}_j)+\sum_{i\neq j}\frac{e^2}{r_{ij}}, \tag{1}$$

where $H(i)$ is the kinetic energy of nucleon i and may also contain a spin-orbit interaction, $V(\mathbf{r}_i-\mathbf{r}_j)$ is the nucleon-nucleon interaction, and e^2/r_{ij} the Coulomb interaction between protons. $V(\mathbf{r}_i-\mathbf{r}_j)$ is to be summed over all pairs of nucleons while e^2/r_{ij} is to be summed over all pairs of protons. The wave function of the nucleus is taken to be

$$\Psi=\text{determinant}\left|\prod_i \phi_m(\mathbf{r}_i,\boldsymbol{\sigma}_i,\boldsymbol{\tau}_i)\right|, \tag{2}$$

$$\phi_m(\mathbf{r}_i,\boldsymbol{\sigma}_i,\boldsymbol{\tau}_i)=\psi_m(\mathbf{r}_i)\chi_m(\boldsymbol{\sigma}_i)\zeta_m(\boldsymbol{\tau}_i), \tag{3}$$

i.e., a determinant formed from the products of single-nucleon wave functions $\phi_n(\mathbf{r}_i,\boldsymbol{\sigma}_i,\boldsymbol{\tau}_i)$ which are in turn the products of a space-part $\psi_m(\mathbf{r}_i)$, a spin part $\chi_m(\boldsymbol{\sigma}_i)$, and an isotopic spin part $\zeta_m(\boldsymbol{\tau}_i)$. The subscript m indicates the quantum numbers. In the present work, we shall assume the shell structure and assign the spin and the angular momentum quantum numbers to the various nucleons in accordance with the Pauli principle; but we shall leave the radial dependence of $\psi_m(\mathbf{r}_i)$ to be determined by the variational principle.

The potential $V(\mathbf{r}_i-\mathbf{r}_j)$, as discussed below, is considered to have an unknown parameter, say the strength factor V_0. The wave functions $\psi_m(\mathbf{r}_i)$ and the parameter V_0 are to be determined by the variational principle

$$\delta E=\delta\int \Psi^* H\Psi dq=0, \tag{4}$$

together with the requirement that the total energy E of the nucleus be equal to the empirical value E_0 of the binding energy of the nucleus[5]:

$$\int \Psi^* H\Psi dq=E_0. \tag{5}$$

The variational equation (4) leads to a system of Hartree-Fock equations equal in number to the number of different shells in the nucleus. The solution of this system of coupled differential-integral equations together with (5) will be very difficult in general, and in our present work, we shall solve (4) approximately by

[4] See Sec. VI below.

[5] W. Heisenberg, Z. Physik **96**, 1421 (1935).

the modified Ritz method so familiar in atomic and molecular problems. The $\psi_m(r)$ are given reasonable analytic forms with variable parameters, say $\nu_1, \cdots, \nu_k$. Equations (4) and (5) are then a system of $k+1$ equations:

$$\partial E/\partial \nu_i = 0, \quad i=1, \cdots k; \quad E(\nu_1, \cdots, \nu_k) = E_0, \quad (6)$$

for the $k+1$ unknowns $\nu_1, \cdots \nu_k$, V_0.

For the nucleon-nucleon potential $V(\mathbf{r}_i - \mathbf{r}_j)$, we shall ignore tensor forces in the present preliminary approach and assume a general combination of Wigner, Majorana, Bartlett, and Heisenberg interactions having the same central field dependence:

$$V(|\mathbf{r}_i - \mathbf{r}_j|) = (a_W + a_M P_M + a_B P_B + a_H P_H) J(r_{ij}) \quad (7)$$

It would have been most satisfactory if there existed an interaction $V(\mathbf{r}_i - \mathbf{r}_j)$ for two "free" nucleons in the sense of the Coulomb interaction between electrons in the atomic problem. It is known, however, that no single $V(\mathbf{r}_i - \mathbf{r}_j)$ succeeds in accounting for all the known data (deuteron, low and high energy scatterings) for the two-nucleon systems. As we are not concerned with very high nucleon energies in a nucleus, we shall choose $V(\mathbf{r}_i - \mathbf{r}_j)$ to be consistent with such low-energy data as (i) the binding energy of the deuteron, (ii) the cross sections of the slow neutron proton scattering, and (iii) the effective ranges as determined by these scattering data. Furthermore, for the central field $J(r_{ij})$, we shall assume the Yukawa potential

$$J(r_{ij}) = V_0 e^{-x}/x, \quad x = r_{ij}/r_0, \quad (8)$$

where V_0 and r_0 are adjustable constants. Other forms of $J(r_{ij})$ can be used, (8) being chosen only for definiteness. V_0 in (8) is defined to be negative in the following.

Now, from (7) and (8), one finds for the triplet-even and singlet-even states the potential

$$\begin{aligned} {}^3V^{\text{even}}(r_{ij}) &= (a_W + a_M + a_B + a_H) J(r_{ij}) \\ &= {}^3A\ V_0 e^{-x}/x, \\ {}^1V^{\text{even}}(r_{ij}) &= (a_W + a_M - a_B - a_H) J(r_{ij}) \\ &= {}^1A\ V_0 e^{-x}/x. \end{aligned} \quad (9)$$

Analysis of the experimental data (i), (ii), and (iii) shows that, with the Yukawa potential (8), the value of r_0 is different for the triplet-even and the singlet-even states, namely[6]

$$\begin{aligned} {}^3V^{\text{even}}&: \quad r_0 \cong 1.4 \times 10^{-13} \text{ cm}, \\ {}^1V^{\text{even}}&: \quad r_0 \cong 1.08 \times 10^{-13} \text{ cm}, \end{aligned} \quad (10)$$

and for $r_0 = 1.4 \times 10^{-13}$ cm, $\frac{1}{2}({}^3A + {}^1A) V_0 \simeq -46$ Mev. Without attempting to fit the two data (10) in our $V(r_i - r_j)$, nor the empirical values of the strength factor ${}^3A\ V_0$ and ${}^1A\ V_0$, we shall merely employ one single Yukawa potential (8) in (7), (i.e., one single value of r_0) and the relations (9). It turns out in the following that only the combination $({}^3A + {}^1A) V_0$ appears in the variational problem which determines $({}^3A + {}^1A) V_0$ as a function of the value a_W whose choice is at our disposal. (See Sec. III, Table I.)

We shall further narrow down the arbitrary choice of the coefficients in (7) by assuming that the interaction $V(r_i - r_j)$ vanishes for the singlet-odd states,[7] namely

$${}^1V^{\text{odd}}(r_{ij}) = (a_W - a_M - a_B + a_H) V_0 e^{-x}/x = 0. \quad (11)$$

This assumption is admittedly arbitrary, it having been made for the purpose of representing to some extent the high symmetry in the observed angular distribution of proton-neutron scattering at ~ 100 Mev about the scattering angle $\vartheta \simeq \pi/2$ in the center-of-mass system, and yet without sacrificing the possibility of meeting the saturation requirement by making $V(\mathbf{r}_i - \mathbf{r}_j)$ vanish also for the triplet-odd states, as in Serber's potential. The relations (9) and (11) enable three of the four coefficients in (7) to be expressed in terms of the fourth. Thus, we may write

$$\begin{aligned} a_M &= \tfrac{1}{2}({}^3A + {}^1A) - a_W, \\ a_H &= \tfrac{1}{2}({}^3A) - a_W, \\ a_B &= -\tfrac{1}{2}({}^1A) + a_W. \end{aligned} \quad (12)$$

We shall finally require the potential $V(|\mathbf{r}_i - \mathbf{r}_j|)$ to satisfy the requirement of saturation of nuclear forces, which is expressed by some well-known relations among the a's.[8] On combining these relations with (12), one obtains the following condition:

$$a_W V_0 \geq \tfrac{1}{6}({}^3A + {}^1A) V_0. \quad (13)$$

V_0 has been defined as negative in (8). We shall denote by b and a_W'

$$b = \tfrac{1}{2}({}^3A + {}^1A), \quad a_W' = a_W/b. \quad (14)$$

The condition (13) becomes then

$$a_W' \leq \tfrac{1}{3}. \quad (15)$$

We wish to emphasize here that the specific assumptions (8), (10), (11), or even the saturation condition are not an inherent part of our main thesis. They have been made merely to enable a definite calculation to be carried out in the present work, which is a preliminary exploratory step in our general program. One might object that the Yukawa potential (8) does not contain the repulsive core indicated both by the high-energy nucleon scattering data and by the meson field theoretical considerations. It may be pointed out, however, that as long as one works in the central-field approximation represented by (3), there is no difficulty in introducing a repulsive core represented by an

[6] E. E. Salpeter, Phys. Rev. **82**, 60 (1951); G. E. Tauber and T. Y. Wu, Phys. Rev. **94**, 1307 (1954).

[7] A. B. Bhatia and S. M. Shah (to be published). We are grateful to Dr. Bhatia for letting us see his manuscript before publication.

[8] See J. M. Blatt and V. Weisskopf, *Theoretical Nuclear Physics* (John Wiley and Sons, Inc., New York, 1952).

inverse power law not steeper than $1/r^2$. The energy of the system is expressible in terms of Slater integrals of the form (21) below; and these integrals can be transformed into integrals of the form $\int_0^\infty \Phi(r)J(r)dr$, $r=r_{ij}$ [of which the Talmi integrals (24) below are a special case corresponding to the oscillator wave functions (19)]. Such integrals are convergent if $J(r)$ in (7) is not more singular than $1/r^2$.

We have not introduced such repulsive cores in $J(r_{ij})$ mainly for reason of simplicity. This may be justified since in the nuclear model we are not dealing with high-energy nucleons, and for low energies the effect of a repulsive core is not important. In any case, modifications and refinements of our specific assumptions such as (8), (10), and (11) can be made if desired and warranted on the basis of the result of the present work.

III. V_0 AND $\psi_m(r_i)$ FROM A MODIFIED RITZ METHOD: O^{16} NUCLEUS

The space and the spin part of the single-nucleon wave function (3) can be put either in the m_l, m_s representation,

$$\psi(n,l,m_l;r)\chi(m_s;\sigma)=(1/r)R_{nl}(r)Y_{l,m_l}(\vartheta,\varphi)\chi(m_s;\sigma), \tag{16}$$

which is appropriate for the case of L, S coupling, or in the J, M representation in the form of linear combinations

$$\sum_{l,m_l} c_{lm_l}{}^{JM}\psi(n,l,m_l;r)\chi(m_s;\sigma) \tag{17}$$

which is appropriate for the case of strong spin-orbit coupling. For the present purpose, we shall neglect the spin-orbit interactions and shall employ the form (16).

For the O^{16} nucleus, the nucleon configurations are $(1s^2)_N(1p^6)_N(1s^2)_P(1p^6)_P$. On account of the presence of the Coulomb interactions between protons in (1), the $1s$ wave functions are different for the neutrons and the protons, and similarly for the $1p$ wave functions, even though the nucleon-nucleon potential $V(|\mathbf{r}_i-\mathbf{r}_j|)$ is assumed to be charge independent. Thus there are 4 different orbitals $(1s)_N$, $(1p)_N$, $(1s)_P$, $(1p)_P$ which are given by (4), or the Hartree-Fock equations. As mentioned before, we shall solve (4) by the usual modified form of Ritz method, and on account of the analytical complexity involved in the calculation, we shall as a first approximation assume for the radial functions $R_{nl}(r)$ in (16) the analytic form of the wave function of a 3-dimensional harmonic oscillator, namely,[9]

$$R_{nl}(r)=N_{nl}(\nu_{nl})\exp(-\tfrac{1}{2}\nu_{nl}r^2)r^{l+1}L_{n+l+\frac{1}{2}}{}^{l+\frac{1}{2}}(\nu_{nl}r^2), \tag{18}$$
$$\pi^{\frac{1}{2}}n![(2l+1)!!]^2N_{nl}{}^2(\nu_{nl})=2^{l-n+2}(2l+2n+1)!!\nu_{nl}{}^{l+\frac{3}{2}},$$

where n,l are the radial and azimuthal quantum numbers respectively, L is the associated Laguerre polynomial, and ν_{nl} is a constant regarded as a variational parameter, to be determined by (6). One should employ different ν_{nl} for the proton and the neutron on account of the Coulomb interaction, but as a simplifying approximation in the present exploratory work, we shall ignore the difference in the wave functions of the neutron and the proton, although the energy contribution from the Coulomb interaction e^2/r_{ij} in (1) is included.

To obtain the energy integral in (4), we note that with the use of the wave function (18), the diagonal matrix element of the one-particle Hamiltonian $H(i)=(1/2M)p_i{}^2$ is simply

$$\langle n,l|H(i)|n,l\rangle=(\tfrac{3}{2}+2n+l)(\hbar^2/2M)\nu_{nl}, \tag{19}$$

so that for the 16 nucleons $(1s^2)_N(1p^6)_N(1s^2)_P(1p^6)_P$ the kinetic energy part of the energy integral (4) is

$$T=(3\nu_0+15\nu_1)(\hbar^2/M), \tag{20}$$

where ν_0 and ν_1 are the variational parameters for the $1s$ and $1p$ wave functions in (18) respectively.

The matrix element of the potential energy terms in (1) can be shown to be expressible in terms of the following generalized Slater integrals:

$$F^k(n,n')=\int_0^\infty\int_0^\infty R_n{}^2(r_1)R_{n'}{}^2(r_2)w_k(r_1,r_2)dr_1dr_2, \tag{21}$$

$$G^k(n,n')=\int_0^\infty\int_0^\infty R_n(r_1)R_n(r_2)R_{n'}(r_1)\times R_{n'}(r_2)w_k(r_1,r_2)dr_1dr_2, \tag{22}$$

$$w_k(r_1,r_2)=\frac{2k+1}{2}\int_{-1}^{1}J(r_{12})P_k(\cos\Theta)d\cos\Theta,$$

where Θ is the angle between r_1 and r_2, and similar integrals $f^k(n,n')$, $g^k(n,n')$ in which $w_k(r_1,r_2)$ is given by (22) with $J(r_{12})$ of (7) replaced by the Coulomb potential. $P_k(\cos\Theta)$ is the Legendre polynomial.

With the use of the determinantal wave function (2), each type of the potential $V(|\mathbf{r}_1-\mathbf{r}_2|)$ in (7) gives rise to a "direct" and an "exchange" integral. The matrix elements of each type of interaction in $\sum_{i\neq j}V(|\mathbf{r}_i-\mathbf{r}_j|)$ for all nucleons and of $\sum e^2/r_{ij}$ in the O^{16} nucleus are

[9] I. Talmi, Helv. Phys. Acta, **25**, 185 (1952). The use of harmonic oscillator wave functions in our present work is of course mainly for reason of simplicity. The rapid decrease with distance as given by the factor $\exp(-\frac{1}{2}\nu_{nl}r^2)$ seems preferable to the use of hydrogenic wave functions, when considered in the light of the short-range nature of the "central field" both expected and obtained in Sec. VII below. Eventually one may replace the simple functions (18) by combinations of R_{nl} for different n but the same l. They may be regarded as the wave functions of an anharmonic isotropic oscillator.

given below.

$$
\begin{aligned}
&a_W \sum_{i\neq j} \int \Psi^* J(r_{ij}) \Psi dq \\
&\quad = a_W[6F^0(0,0)+48F^0(0,1)-4G^1(0,1) \\
&\qquad +66F^0(1,1)-(12/5)F^2(1,1)], \\
&a_M \sum_{i\neq j} \int \Psi^* P_M J(r_{ij}) \Psi dq \\
&\quad = a_M[6F^0(0,0)-12F^0(0,1)+16G^1(0,1) \\
&\qquad +6F^0(1,1)+(48/5)F^2(1,1)], \\
&a_B \sum_{i\neq j} \int \Psi^* P_B J(r_{ij}) \Psi dq \\
&\quad = a_B[24F^0(0,1)-8G^1(0,1) \\
&\qquad +24F^0(1,1)-(24/5)F^2(1,1)], \\
&a_H \sum_{i\neq j} \int \Psi^* P_H J(r_{ij}) \Psi dq \\
&\quad = -a_H[24F^0(0,1)-8G^1(0,1) \\
&\qquad +24F^0(1,1)-(24/5)F^2(1,1)], \\
&\sum_{i\neq j}^{\text{protons}} \int \Psi^* \frac{e^2}{r_{ij}} \Psi dq \\
&\quad = f^0(0,0)+12f^0(0,1)-2g^1(0,1) \\
&\qquad +15f^0(1,1)-(6/5)f^2(1,1).
\end{aligned} \tag{23}
$$

Here and below, we denote the $1s$, $1p$, $1d$ state by the "collective" quantum number 0, 1, 2, respectively.

In the present approximation, if one uses the simple harmonic oscillator wave functions (18), all the integrals F^k, G^k, f^k, g^k in (21) can be expressed in terms of the integrals[10]

$$
\begin{aligned}
I_l(\nu_l) &= N_l^2(\nu_l/2) \int_0^\infty \exp(-\tfrac{1}{2}\nu_l r^2) r^{2l+2} J(r) dr, \\
g_l(\nu_l) &= e^2 N_l^2(\nu_l/2) \int_0^\infty \exp(-\tfrac{1}{2}\nu_l r^2) r^{2l+1} dr,
\end{aligned} \tag{24}
$$

where $J(r)$ is given by (18). Thus

$$
\begin{aligned}
&F^0(0,0) = I_0(\nu_0), \\
&F^0(1,1) = G^0(1,1) = (1/12)[5(I_0(\nu_1)+I_2(\nu_1))+2I_1(\nu_1)], \\
&F^2(1,1) = G^2(1,1) = (25/12)[I_0(\nu_1)+I_2(\nu_1)-2I_1(\nu_1)], \\
&G^1(0,1) = 24(\nu_0^3\nu_1^5)^{\frac{1}{4}}(\nu_0+\nu_1)^{-4}[I_0(\bar{\nu})-I_1(\bar{\nu})], \\
&F^0(0,1) = (\nu_0+\nu_1)^{-1}[\nu_1 I_0(\bar{\nu})+\nu_0 I_1(\bar{\nu})], \\
&\qquad \bar{\nu} = 2\nu_0\nu_1/(\nu_0+\nu_1),
\end{aligned} \tag{25}
$$

and similar expressions for the Coulomb part f^k, g^k, with g_l replacing I_l in (25).

The Talmi integrals (24) can be evaluated for certain potentials $V(r)$. For the Yukawa potential (8), one finds[10]

$$
\begin{aligned}
&\mu = 1/[r_0(2\nu)^{\frac{1}{2}}], \\
&I_0(\nu) = C(\mu) - D(\mu), \\
&I_1(\nu) = \tfrac{2}{3}(1+\mu^2)C(\mu) - (1+\tfrac{2}{3}\mu^2)D(\mu), \\
&I_2(\nu) = (8/15)[1+(9/4)\mu^2+\tfrac{1}{2}\mu^4]C(\mu) \\
&\qquad -[1+(4/3)\mu^2+(4/15)\mu^4]D(\mu), \\
&I_3(\nu) = (16/35)[1+(29/8)\mu^2+(5/3)\mu^4+\tfrac{1}{6}\mu^6]C(\mu) \\
&\qquad -[1+2\mu^2+\tfrac{4}{5}\mu^4+(8/105)\mu^6]D(\mu), \\
&g_l(\nu) = \frac{e^2}{r_0\mu(\pi)^{\frac{1}{2}}} \frac{2^l l!}{1\cdot 3\cdot 5\cdots(2l+1)}, \\
&C(\mu) = V_0/(\mu\pi^{\frac{1}{2}}), \\
&D(\mu) = V_0[1-\Phi(\mu)]\exp(\mu^2), \\
&\Phi(\mu) = \frac{2}{\pi^{\frac{1}{2}}} \int_0^\mu \exp(-t^2) dt.
\end{aligned} \tag{26}
$$

By means of (23) and (26), one obtains for the total energy of the O^{16} nucleus:

$$
\begin{aligned}
E(O^{16}) = &(3\nu_0+15\nu_1)\hbar^2/M+6(a_W+a_M)I_0(\nu_0) \\
&+12(4a_W-a_M+2a_B-2a_H)F^0(0,1) \\
&-4(a_W-4a_M+2a_B-2a_H)G^1(0,1) \\
&+(45/2)(a_W+a_M)[I_0(\nu_1)+I_2(\nu_1)] \\
&+3(7a_W-13a_M+8a_B-8a_H)I_1(\nu_1) \\
&+g_0(\nu_0)+12f^0(0,1)-2g^1(0,1)+(43/4)g_0(\nu_1).
\end{aligned} \tag{27}
$$

It is to be noted that this expression follows from (1) and the potential (7), and is independent of any of the specific assumptions (10), (11), and (15). We shall now use (12) and (14), and absorb the factor b in the as yet undetermined V_0 by replacing the V_0 in all the Talmi integrals I_l in (24), (27), by V_0', where

$$
V_0' = bV_0. \tag{28}
$$

Equation (27) can then be written in the form

$$
\begin{aligned}
E(O^{16}) = &(3\nu_0+15\nu_1)\hbar^2/M+6I_0(\nu_0)+AF^0(0,1) \\
&+BG^1(0,1)+CI_1(\nu_1)+(45/2)[I_0(\nu_1)+I_2(\nu_1)] \\
&+g_0(\nu_0)+12f^0(0,1)-2g^1(0,1)+(43/4)g_0(\nu_1),
\end{aligned} \tag{27a}
$$

$$
A = 36(3a_W'-1), \quad B = 12(2-3a_W'), \quad C = 9(12a_W'-7). \tag{29}
$$

The empirical value of $E(O^{16})$ is taken to be -127.56 Mev.

For the variational equations (6), we make use of

[10] I. Talmi, reference 9; G. E. Tauber and T. Y. Wu, Phys. Rev. **94**, 1307 (1954). It is important to note that the integrals I_l and g_l in (24) refer not to the wave functions (19) but to normalized wave functions obtained by replacing ν by $\frac{1}{2}\nu$ in (19). Thus all the integrals I_l in Talmi's paper should have ν replaced by $\frac{1}{2}\nu$. While this amounts only to a redefinition of ν in Talmi's paper and is inconsequential, this is important in the present work since the matrix elements of the kinetic energies contain ν.

the following recurrence formulas:

$$\frac{\partial I_l(\nu)}{\partial \nu}=\frac{3+2l}{2\nu}[I_l(\nu)-I_{l+1}(\nu)], \qquad \frac{\partial g_l(\nu)}{\partial \nu}=\frac{1}{2\nu}g_l(\nu). \tag{30}$$

Equation (6) leads to

$$\frac{6\hbar^2\nu_0}{M}+18[I_0(\nu_0)-I_1(\nu_0)]+\frac{3A\bar{\nu}^2}{4\nu_0^2\nu_1}[(3\nu_1-2\nu_0)I_0(\bar{\nu})+(7\nu_0-3\nu_1)I_1(\bar{\nu})-5\nu_0 I_2(\bar{\nu})]$$
$$+\frac{3B\bar{\nu}^5}{4(\nu_0^7\nu_1^3)^{\frac{1}{2}}}\left[11I_0(\bar{\nu})-16I_1(\bar{\nu})+5I_2(\bar{\nu})-10\frac{\nu_0}{\bar{\nu}}[I_0(\bar{\nu})-I_1(\bar{\nu})]\right]$$
$$+g_0(\nu_0)+3\left(\frac{\bar{\nu}}{\nu_0}\right)^2 g_0(\bar{\nu})-\frac{\bar{\nu}^5(4\nu_1-5\nu_0)}{2(\nu_0^7\nu_1^5)^{\frac{1}{2}}}g_0(\bar{\nu})=0, \tag{31a}$$

$$\frac{30\hbar^2\nu_1}{M}+\frac{5A\bar{\nu}^2}{4\nu_0\nu_1^2}[\nu_1 I_0(\bar{\nu})+(\nu_0-\nu_1)I_1(\bar{\nu})-\nu_0 I_2(\bar{\nu})]+5C[I_1(\nu_1)-I_2(\nu_2)]+\frac{3B\bar{\nu}^5}{4(\nu_0\nu_1)^{5/2}}\left[11I_0(\bar{\nu})-16I_1(\bar{\nu})\right.$$
$$\left.+5I_2(\bar{\nu})-6\frac{\nu_1}{\bar{\nu}}[I_0(\bar{\nu})-I_1(\bar{\nu})]\right]+\frac{45}{2}\{3[I_0(\nu_1)-I_1(\nu_1)]+7[I_2(\nu_1)-I_3(\nu_1)]\}+\frac{43}{4}g_0(\nu_1)$$
$$+6\left(\frac{\bar{\nu}}{\nu_0}\right)^2\left[1-\frac{5\nu_1}{6\nu_0}-\frac{\bar{\nu}^3(2\nu_0-\nu_1)}{4(\nu_0^7\nu_1)^{\frac{1}{2}}}\right]g_0(\bar{\nu})=0. \tag{31b}$$

Equations (27a), (31a), and (31b) are three equations in the three unknowns V_0', ν_0, and ν_1 with a_W' as a parameter. For each choice of a_W' which is still at our disposal and is subject only to the saturation requirement (15), Eqs. (27a), (31a), and (31b) give a set of values for V_0', ν_0, and ν_1. Table I gives the solution of these three equations for

$$a_W'=\tfrac{1}{3}, \quad r_0=1.4\times10^{-13}\text{ cm}, \tag{32}$$

and the solutions for $a_W'=0.3$, 0.22 and the same r_0 but with the further approximation $\nu_1=\nu_0$. The value $bV_0\simeq-54$ Mev is to be compared with the value -46 Mev in (10) for two "free" nucleons.

Other choices of a_W' and r_0 are obviously possible, and trial wave functions more general then (19) should be used. In the present preliminary work, however, we intend to bring out the general features of the variational treatment. Since any calculation must necessarily be based on an assumed pair interaction such as (7) and (8), it does not seem warranted to carry out very long calculations at this stage.[11]

IV. TOTAL BINDING ENERGY OF O^{15} AND O^{17} NUCLEI

We shall calculate the total binding energy of O^{15} by means of the assumption that the potential $V(|r_i-r_j|)$ in O^{15} is the same as that determined for O^{16} in the preceding section, and the further approximation that the wave functions for the $1s$ and $1p$ nucleons in O^{15} are also nearly the same as those in O^{16}. Thus for the configuration $(1s^2)_N(1p^5)_N(1s^2)_P(1p^6)_P$, the expressions for the kinetic and the potential energy in (20) and (23) are replaced by

$$T=\frac{\hbar^2}{M}\left(3\nu_0+\frac{55}{4}\nu_1\right), \tag{20-B}$$

and

$$a_W[6F^0(0,0)+44F^0(0,1)-(11/3)G^1(0,1)$$
$$+55F^0(1,1)-2F^2(1,1)]+a_M[6F^0(0,0)-11F^0(0,1)$$
$$+(44/3)G^1(0,1)+5F^0(1,1)+8F^2(1,1)]$$
$$+(a_B-a_H)[22F^0(0,1)-(22/3)G^1(0,1)+20F^0(1,1)$$
$$-4F^2(1,1)]+f^0(0,0)+12f^0(0,1)-2g^1(0,1)$$
$$+15f^0(1,1)-(6/5)f^2(1,1). \tag{23-B}$$

The expression for the energy $E(O^{15})$ corresponding to (27a) for O^{16} can be written down. Again, we shall make the choice $a_W'=\frac{1}{3}$ as in (33), and with the values $\mu_0=0.5808$, $\mu_1=0.5650$, $V_0'=bV_0=-54$ Mev in Table I obtained by the variational calculation for O^{16}, we find

TABLE I. Variational calculation for O^{16}.[a]

a_W'	r_0 cm	μ_0	μ_1	$V_0'=bV_0$ Mev
1/3	1.4×10^{-13}	0.5808	0.5650	−54
0.3	1.4×10^{-13}	0.60		−60
0.22	1.4×10^{-13}	0.70		−75

[a] See (8), (14), (18), (26), (28) for definition of the various quantities.

[11] A calculation similar to that described here has been carried out by M. G. Redlich [Phys. Rev. **99**, 1421 (1955)] for O^{16}. The main difference between his work and the present work is that he uses an explicit harmonic oscillator potential V' for the central potential and then calculates the binding energy, while we use the empirical value of the binding energy to fix the constant V_0 of the two-body interaction and make no assumption about the central potential, which is obtained from the Hartree-Fock equations (see Secs. V and VII).

TABLE II. Variational calculation for O^{15}. (Compare with Table I.)

a_W'	μ	bV_0 (Mev)
1/3	0.56	−56.3
0.3	0.60	−61.5

for $E(O^{15})$ the value

$$E(O^{15})=-88.1 \text{ Mev},$$

which is much too small compared with the empirical value −111.97 Mev. We have also calculated $E(O^{15})$ corresponding to $a_W'=0.3$, $a_W'=0.22$, and $\mu_0=\mu_1$ in Table I, and found $E(O^{15})=-96.80$, −95.01 Mev respectively. The agreement with the empirical value is only partly improved.

A part of the discrepancy noted above obviously can arise from insufficient variations in the range of the trial values for a_W' and from the nature of approximation introduced by the use of the wave functions (18). Also the Talmi integrals $I_l(\nu)$ in (26) appearing in the energy expressions, and hence the energy values (for O^{16} and O^{15}), depend very sensitively on the parameters ν_l. Hence the above comparison between the calculation $E(O^{15})$ and the empirical value may not be a fair test. We have, therefore, inverted the test by calculating the O^{15} problem by an independent variational calculation similar to that for O^{16}, and compare the solutions μ, bV_0 so obtained with those of O^{16} in Table I. With the empirical value $E(O^{15})=-111.97$ Mev and $\nu_0=\nu_1$, the result of solving (27a-B) with the following variational equation [see remark before (28)]

$$\begin{aligned}&(67\hbar^2\nu/2M)+3A'I_0(\nu)+(5B'-3A')I_1(\nu)\\&+(7C'-5B')I_2(\nu)-7C'I_3(\nu)+(83/4)\mathcal{I}_0(\nu)=0, \quad \text{(31-B)}\\&A'=165/4, \quad B'=(189a_W'-102), \quad C'=75/4,\end{aligned}$$

is given in Table II.

A comparison of Table II and Table I shows that for the same value of a_W' the variational calculation leads to very much the same wave functions and very nearly the same potential bV_0 for the pair-interaction in O^{15} and O^{16}. One can conclude from this that the fundamental ideas of this model (namely, a central-field approximation starting from a pair-interaction between two nucleons) have at least not been contradicted by this test.

For O^{17}, we have an additional $1d$ neutron, and the total energy is obtained by adding to (20) and (23) terms arising of this $1d$ neutron namely,

$$\begin{aligned}E(O^{17})=&E(O^{16}) \text{ in (27}a\text{)}+(7\hbar^2\nu_2/4M)\\&+(4a_W+2a_B-a_M-2a_H)[F^0(2,0)+3F^0(2,1)]\\&+(4a_M+2a_H-2a_B-a_W)[\tfrac{1}{5}G^2(2,0)\\&+\tfrac{2}{5}G^1(2,1)+(9/35)G^3(2,1)], \quad \text{(27-A)}\end{aligned}$$

where ν_2 is the parameter in (18) for the $1d$ wave function, and the F's and G's are given by (21).

Two calculations have been made. (*i*) With the V_0' and the parameters ν_0, ν_1 for the $1s$, $1p$ nucleons which have already been determined for O^{16} (Table I), the parameter $\nu_2(1d)$ and $E(O^{17})$ in (27-A) are calculated from the variational equation. (*ii*) With the ν_0, ν_1 for O^{16} from Table I and the empirical value of $E(O^{17})=-131.66$ Mev, the parameter $\nu_2(1d)$ and V_0' are calculated. In each case the limiting value $a_W'=\frac{1}{3}$ and (12) have been used. The calculation (*i*) gives

$$\mu_2(1d)=0.585, \quad E(O^{17})=-116.77 \text{ Mev}, \quad \text{(33a)}$$

while calculation (*ii*) gives

$$\mu_2(1d)=0.584, \quad V_0'=-55.2 \text{ Mev}. \quad \text{(33b)}$$

It is seen that the same remarks above for O^{15} hold here for O^{17}.

V. HARTREE-FOCK EQUATIONS (FOR O^{16}, O^{15}, O^{17} NUCLEI IN PARTICULAR)[12]

The variational equation (4) with the assumption (2) is equivalent to the following system of Fock equations

$$\begin{aligned}&[H(i)+V(i)-G_{nn}(i)-\lambda_n']\phi_n(i)\\&\qquad=\textstyle\sum_m{}'[G_{mn}(i)+L_{mn}]\phi_n(i). \quad \text{(34)}\end{aligned}$$

Here and in the following, the single index i stands for the set of space, spin, and isotopic spin variables $\mathbf{r}_i$, $\boldsymbol{\sigma}_i$, $\boldsymbol{\tau}_i$ and the index n or m stands for the totality of quantum numbers (of the one-particle state) in (3). $H(i)$ is the one-nucleon Hamiltonian nucleon i in (1), and

$$\begin{aligned}&(m|H(j)|n)=\int\phi_m^*(j)H(j)\phi_n(j)dj,\\&G_{mn}(i)=\int\phi_n^*(j)V(|\mathbf{r}_i-\mathbf{r}_j|)\phi_n(j)dj,\\&V(i)=\textstyle\sum_m G_{mm}(i), \quad \text{(35)}\\&(mk|G|nl)=\int\phi_m^*(i)\phi_k^*(j)V(|\mathbf{r}_i-\mathbf{r}_j|)\\&\qquad\qquad\times\phi_n(i)\phi_l(j)di\,dj,\\&L_{mn}=(m|H(j)|n)\\&\qquad+\textstyle\sum_l[(lm|G|ln)-(lm|G|nl)].\end{aligned}$$

The prime in the summation sign in (34) indicates exclusion of state $m=n$.

On multiplying (34) by the complex conjugate of the spin, isotopic spin, and the space angular part of $\phi_n(i)$, i.e., $\chi_n^*(\boldsymbol{\sigma}_i)\zeta_n^*(\boldsymbol{\tau}_i)Y_n^*(\vartheta_i,\varphi_i)$ in (3) and (18), and summing or integrating over these variables $\boldsymbol{\sigma}_i$, $\boldsymbol{\tau}_i$, ϑ_i, φ_i, one obtains the radial equations for $R_n(r_i)$

[12] Recently M. Rotenberg [Phys. Rev. **100**, 439 (1955)] has carried out a calculation for a 184-nucleon ($Z=N=92$) nucleus in which the Hartree-Fock equations are solved with a Slater average of the exchange term. The charge and particle density distributions are calculated.

of (18):

$$[H_n(r_i)+V(r_i)-\lambda_n]R_n(r_i)$$
$$=\sum_m \alpha_m[\sum_k d^k(n,m)V^k(n,m;r_i)]R_m(r_i), \quad (36)$$

where

$$H_n(r_i)=-\frac{\hbar^2}{2M}\left[\frac{d^2}{dr_i^2}-\frac{l_n(l_n+1)}{r_i^2}\right],$$
$$\lambda_n=\lambda_n'-(n|H(j)|n)-\sum_l[(ln|G|ln)-(ln|G|nl)], \quad (37)$$
$$d^k(n,m)=\int\int Y_n^*(\vartheta_i,\varphi_i)Y_m^*(\vartheta_j,\varphi_j)P_k(\cos\Theta)\times Y_n(\vartheta_i,\varphi_j)Y_n(\vartheta_j,\varphi_j)d\omega_i d\omega_j,$$
$$d\psi_i=\sin\vartheta_i d\vartheta_i d\varphi_i, \quad \text{etc.},$$

P_k being the Legendre polynomial and Θ the angle between $\mathbf{r}_i$ and $\mathbf{r}_j$. α_m is a constant obtained from the coefficients a_d, etc., in the expression (7) or (8) for the potential $V(|\mathbf{r}_i-\mathbf{r}_j|)$.

Before going on further, we shall bring out explicitly in (37) the distinction between the radial wave functions of the neutrons and the protons on account of the Coulomb interactions e^2/r_{ij} in (1). Let us denote the neutron wave functions by $R_n(r)$ and those of the protons by $S_n(r)$. The $V^k(n,m;r)$ are integrals defined by

$$V_{\nu\nu}^k(n,m;r_i)=\int R_n(r_j)R_m(r_j)w_k(r_{ij})dr_j=V_{\nu\nu}^k(m,n;r_i),$$
$$V_{\nu\pi}^k(n,m;r_i)=\int R_n(r_j)S_m(r_j)w_k(r_{ij})dr_j=V_{\pi\nu}^k(m,n;r_i), \quad (38)$$
$$V_{\pi\pi}^k(n,m;r_i)=\int S_n(r_j)S_m(r_j)w_k(r_{ij})dr_j=V_{\pi\pi}^k(m,n;r_i),$$

where $w_k(r_{ij})$ is defined in (22). The subscripts ν, π denote a neutron and a proton respectively. For the protons, there are additional similarly defined integrals:

$$U^k(n,m;r_i)=\int S_n(r_j)S_m(r_j)\omega_k(r_{ij})dr_j, \quad (39)$$

in which $\omega_k(r_{ij})$ is obtained from the expression (22) for $w_k(r_{ij})$ by replacing $J(r_{ij})$ by the Coulomb potential e^2/r_{ij}. The integrals V^k are essentially negative [see (10)] while the U^k are essentially positive. For the evaluation of these integrals, see Appendix.

With this distinction between the neutron and proton, the Fock equations for any given nuclear configuration can be written out. Thus, for the lowest configuration in the O^{16} nucleus, the Fock equations (36) are a system of 4 differential-integral equations in the $1s$ and $1p$ wave functions of the neutrons and the protons. In the following, we shall denote for brevity the $1s$, $1p$, $1d$ state by the single quantum number m or $n=0$, 1, 2 as a subscript respectively, and denotes the eigenvalue parameters for the neutron and proton by λ_m, ϵ_m, respectively. Thus

$$H_0=-\frac{\hbar^2}{2M}\frac{d^2}{dr^2}, \quad H_1=-\frac{\hbar^2}{2M}\left(\frac{d^2}{dr^2}-\frac{2}{r^2}\right),$$
$$H_2=-\frac{\hbar^2}{2M}\left(\frac{d^2}{dr^2}-\frac{6}{r^2}\right), \quad (40)$$

$$[H_0+V_\nu(r)-\lambda_0]R_0(r)=\alpha[V_{\nu\nu}^0(0,0;r)R_0(r)+V_{\nu\nu}^1(0,1;r)R_1(r)]+\beta[V_{\nu\pi}^0(0,0;r)S_0(r)+V_{\nu\pi}^1(0,1;r)S_1(r)], \quad (41\text{-}\nu)$$

$$[H_1+V_\nu(r)-\lambda_1]R_1(r)=\alpha\{\tfrac{1}{3}V_{\nu\nu}^1(0,1;r)R_0(r)+[V_{\nu\nu}^0(1,1;r)+\tfrac{2}{5}V_{\nu\nu}^2(1,1;r)]R_1(r)\}+\beta\{\tfrac{1}{3}V_{\nu\pi}^1(0,1;r)S_0(r)+[V_{\nu\pi}^0(1,1;r)+\tfrac{2}{5}V_{\nu\pi}^2(1,1;r)]S_1(r)\}, \quad (42\text{-}\nu)$$

$$[H_0+V_\pi(r)-\epsilon_0]S_0(r)=[\alpha V_{\pi\pi}^0(0,0;r)+U^0(0,0;r)]S_0(r)+[\alpha V_{\pi\pi}^1(0,1;r)+U^1(0,1;r)]S_1(r)+\beta[V_{\pi\nu}^0(0,0;r)R_0(r)+V_{\pi\nu}^1(0,1;r)R_1(r)], \quad (41\text{-}\pi)$$

$$[H_1+V_\pi(r)-\epsilon_1]S_1(r)=\tfrac{1}{3}[\alpha V_{\pi\pi}^1(0,1;r)+U^1(0,1;r)]S_0(r)+\{\alpha[V_{\pi\pi}^0(1,1;r)+\tfrac{2}{5}V_{\pi\pi}^2(1,1;r)]+U^0(1,1;r)+\tfrac{2}{5}U^2(1,1;r)\}S_1(r)+\beta\{\tfrac{1}{3}V_{\pi\nu}^1(0,1;r)R_0(r)+[V_{\pi\nu}^0(1,1;r)+\tfrac{2}{5}V_{\pi\nu}^2(1,1;r)]R_1(r)\}, \quad (42\text{-}\pi)$$

where

$$\alpha=a_W+\tfrac{3}{2}a_B-a_H-\tfrac{3}{2}a_M,$$
$$\beta=-\tfrac{1}{2}a_H-\tfrac{3}{4}a_M. \quad (43)$$

$$V_\nu(r)=2a_d[V_{\nu\nu}^0(0,0;r)+V_{\pi\pi}^0(0,0;r)+3V_{\nu\nu}^0(1,1;r)+3V_{\pi\pi}^0(1,1;r)], \quad (44)$$

where

$$a_d=a_W+\tfrac{1}{2}(a_B-a_H)-\tfrac{1}{4}a_M,$$
$$V_\pi(2)=V_\nu(r)+2[U^0(0,0;r)+3U^0(1,1;r)]. \quad (45)$$

In general, $V(r)$ can be readily expressed in terms of the integrals (38). It is to be noted that the Eqs. (41) and (42) with α, β given by (43) are perfectly general in the sense that they are independent of such assumptions as (9), (11), and (15) on $V(\mathbf{r}_i-\mathbf{r}_j)$.

For the O^{17} nucleus in the $(1s^2)_N(1p^6)_N(1d)_N(1s^2)_P(1p^6)_P$ configuration, the following terms have to be added to the right-hand side of Eqs. (41-ν), (42-ν),

(41-π), (42-π), respectively:

$$\tfrac{1}{2}\alpha[\tfrac{1}{5}V_{\nu\nu}^{2}(0,2;r)R_2(r)], \quad (41\text{-}\nu\text{-A})$$

$$\tfrac{1}{2}\alpha[(2/15)V_{\nu\nu}^{1}(1,2;r)+(3/35)V_{\nu\nu}^{3}(1,2;r)]R_2(r), \quad (42\text{-}\nu\text{-A})$$

$$\tfrac{1}{2}\beta[\tfrac{1}{5}V_{\pi\nu}^{2}(0,2;r)R_2(r)], \quad (41\text{-}\pi\text{-A})$$

$$\tfrac{1}{2}\beta[(2/15)V_{\pi\nu}^{1}(1,2;r)+(3/35)V_{\pi\nu}^{3}(1,2;r)]R_2(r). \quad (42\text{-}\pi\text{-A})$$

The "equation for the $1d$" neutron is

$$\begin{aligned}[H_2+V_\nu'(r)-\lambda_2]R_2(r)&=\alpha\{\tfrac{1}{5}V_{\nu\nu}^{2}(2,0;r)R_0(r)+[\tfrac{2}{5}V_{\nu\nu}^{1}(2,1;r)\\&+(9/35)V_{\nu\nu}^{3}(2,1;r)]R_1(r)\}+\tfrac{1}{2}\alpha\{V_{\nu\nu}^{0}(2,2;r)\\&+(2/7)V_{\nu\nu}^{2}(2,2;r)+(2/63)V_{\nu\nu}^{4}(2,2;r)\}R_2(r)\\&+\beta\{\tfrac{1}{5}V_{\nu\pi}^{2}(2,0;r)S_0. \quad (43\text{-}\nu\text{-A})\end{aligned}$$

In Eqs. (41-ν-A), (42-ν-A), (43-ν-A) for the neutron and (41-π-A), (42-π-A) for the proton in O^{17}, the $V_\nu(r)$ in (44), (45) is to be reqlaced by

$$V_\nu'(r)=V_\nu(r)+a_dV_{\nu\nu}^{0}(2,2;r). \quad (44\text{-A})$$

For O^{15} in the configuration $(1s^2)_N(1p^5)_N(1s^2)_P(1p^6)_P$ the Fock equations are obtained by *subtracting* the following terms from the right-hand side of (41-ν), (42-ν), (41-π), (42-π) respectively:

$$\tfrac{1}{2}\alpha[\tfrac{1}{3}V_{\nu\nu}^{1}(0,1;r)R_1(r)], \quad (41\text{-}\nu\text{-B})$$

$$\tfrac{1}{2}\alpha\{\tfrac{1}{3}[V_{\nu\nu}^{0}(1,1;r)+\tfrac{2}{5}V_{\nu\nu}^{2}(1,1;r)]R_1(r)\}, \quad (42\text{-}\nu\text{-B})$$

$$\tfrac{1}{2}\beta[\tfrac{1}{3}V_{\pi\nu}^{1}(0,1;r)R_1(2)], \quad (41\text{-}\pi\text{-B})$$

$$\tfrac{1}{2}\beta\{\tfrac{1}{3}[V_{\pi\nu}^{0}(1,1;r)+\tfrac{2}{5}V_{\pi\nu}^{2}(1,1;r)]R_1(r)\}, \quad (42\text{-}\pi\text{-B})$$

where α, β are as given in (43), and the $V_\nu(r)$ in (41-ν-B), (42-ν-B), (41-π-B), (42-π-B) is obtained by replacing $V_\nu(r)$ in (44) and (45) for O^{16} by

$$V_\nu''(r)=V_\nu(r)-a_dV_{\nu\nu}^{0}(1,1;r). \quad (44\text{-B})$$

VI. BINDING ENERGY OF THE "LAST" NUCLEON (OR "IONIZATION POTENTIALS")

For any given nucleus, either the variational equation (2) with the product wave function (2), or the above system of Fock equations, is the complete statement of the central-field approximation. In the form (2), the modified Ritz method so familiar in atomic and molecular problems is convenient; the solution of the Fock equations, while also familiar in atomic and molecular problems, is more easily obtained with the aid of calculating machines. The difficulty in the present nuclear case is the lack of knowledge of the pair-interaction $V(\mathbf{r}_i-\mathbf{r}_j)$, and the consequent necessity for having to explore many assumed forms for $V(\mathbf{r}_i-\mathbf{r}_j)$. The calculations in Secs. III and IV must only be regarded as preliminary explorations illustrating the ideas rather than giving quantitative results. In the same spirit, we shall further discuss some consequences of the central-field approximation.

For this purpose of obtaining only the essential qualitative features of the theory, let us ignore the difference between the neutron and the proton wave functions $R_m(r)$ and $S_m(r)$ in each individual equation, without neglecting the Coulomb interaction entirely. Thus, for example, instead of (41ν), (41π), and (45), we shall consider the following equations for the $1s$ neutron and $1s$ proton in O^{16}:

$$\begin{aligned}[H_0+V_\nu(r)-\lambda_0]R_0(r)&=(\alpha+\beta)[V_{\nu\nu}^{0}(0,0;r)R_0(r)+V_{\nu\nu}^{1}(0,1;r)R_1(r)], \quad (46\nu)\\[H_0+V_\pi(r)-\epsilon_0]S_0(r)&=(\alpha+\beta)[V_{\pi\pi}^{0}(0,0;r)S_0(r)+V_{\pi\pi}^{1}(0,1;r)S_1(r)]\\&+U^0(0,0;r)S_0+U^1(0,1;r)S_1(r), \quad (46\pi)\end{aligned}$$

$$\begin{aligned}V_\nu(r)&=4a_d[V_{\nu\nu}^{0}(0,0;r)+3V_{\nu\nu}^{1}(1,1;r)],\\V_\pi(r)&=4a_d[V_{\pi\pi}^{0}(0,0;r)+3V_{\pi\pi}^{2}(1,1;r)]\\&+2[U^0(0,0;r)+3U^1(1,1;r)].\end{aligned} \quad (47)$$

This approximation simplifies the system of Eqs. (41) and (42) for $R_0(r)$, $R_1(r)$, $S_0(r)$, and $S_1(r)$ into two independent systems, one for $R_0(r)$ and $R_1(r)$, and one for $S_0(r)$ and $S_1(r)$. While an accurate solution of each system for the wave functions and the eigenvalues λ_0, λ_1, ϵ_0, ϵ_1 can be carried out, one may obtain an approximate value of λ_0, for example, by using in (46ν) the approximation variational (normalized) wave functions $R_0(r)$ and $R_1(r)$ obtained by the modified Ritz method in Sec. III.

Equations (46ν) and (46π) can be further simplified if we set $a_d=0$ (44-A) (i.e., $a_W'=\frac{1}{3}$ in Tables I and II). From (43), (14b), and (14), one obtains readily

$$\begin{aligned}\alpha+\beta&=(25/9)a_d-\tfrac{5}{6}({}^3A+{}^1A)=(25/9)a_d-(5/3)b \quad (48)\\&=-(5/3)b \quad \text{for } a_d=0. \quad (48a)\end{aligned}$$

With $a_d=0$, one obtains, for example, from (46ν) and (48),

$$\lambda_0=\int R_0H_0R_0dr+\frac{5}{3}b\int R_0(r)[V_{\nu\nu}^{0}(0,0;r)R_0(r)+V_{\nu\nu}^{1}(0,1;r)R_1(r)]dr. \quad (49)$$

The integrals in (49) and in similar expressions for ϵ_0 ($1s$ proton), λ_1 ($1p$ neutron), ϵ_1 ($1p$ proton) can all be expressed in terms of the Talmi integrals in (26). The resulting expressions are

$$(1s)_N: \quad \lambda_0=\frac{3\hbar^2\nu_0}{4M}+\frac{5}{3}[I_0(\nu_0)+G^1(0,1)], \quad (50)$$

$$(1s)_P: \quad \epsilon_0=\lambda_0-g^1(0,1)+\frac{e^2}{\pi r_0\mu_0}+6f^0(0,1),$$

$$(1p)_N: \quad \lambda_1=\frac{5\hbar^2\nu_1}{4M}+\frac{5}{3}[\tfrac{1}{3}G^1(0,1)+\tfrac{1}{4}\{5I_0(\nu_1)+5I_2(\nu_1)-6I_1(\nu_1)\}], \quad (51)$$

$$(1p)_P: \quad \epsilon_1=\lambda_1-\tfrac{1}{3}g^1(0,1)+2f^0(0,1)+\frac{43e^2}{12\pi r_0\mu_1},$$

where the expressions I_l, $G^1(0,1)$ and $f^0(0,1)$ are given in (25) and (26), with V_0 replaced by $V_0'=bV_0$ as in (27a). With the values of $\mu_0=0.5808$, $\mu_1=0.5650$, $a_W'=\frac{1}{3}$, $V_0'=-54$ Mev, one obtains the result in Table III. These are the approximate binding energy of the "last" $1s$, $1p$ neutron, proton, respectively, in the O^{16} and O^{15} nuclei. The differences between the neutron and the proton energy for the corresponding orbit are due to the Coulomb interactions among the protons.

These binding energies in Table III, especially the positive values for the $1p$ state are seen to be unsatisfactory. It must be remembered, however, that the values of the parameter λ,ϵ in the Fock equations are not exactly the "ionization potentials," which must be obtained from the difference between the energies of the A- and $(A-1)$-nucleon nuclei. Nevertheless, Table III shows that the eigenvalues λ and ϵ of the Fock equations do not give sufficiently good approximate values of the binding energies for the individual nucleons.

VII. CENTRAL FIELD: HARTREE AND FOCK APPROXIMATIONS

All the individual Fock equations (41) and (42) can be regarded as the radial equations of a particle in a central field. Thus, for example, Eq. (41-ν) for the $1s$ neutron may be regarded as an equation of a central field problem

$$[H_0+\mathcal{W}_\nu(r)-\lambda]R_0(r)=0, \tag{52}$$

where the central field $\mathcal{W}_\nu(r)$ is

$$\mathcal{W}_\nu(r)=V_\nu(r)-\alpha V_{\nu\nu}{}^0(0,0;r)$$
$$-\frac{1}{R_0(r)}[\alpha V_{\nu\nu}{}^1(0,1;r)R_1(r)+\beta V_{\nu\pi}{}^0(0,0;r)S_0(r)$$
$$+\beta V_{\nu\pi}{}^1(0,1;r)S_1(r)]. \tag{53}$$

This field $\mathcal{W}_\nu(r)$ is obviously different for the various shells $(1s)_N$, $(1p)_N$, etc. On the other hand, the usual treatment of the shell model implies an average central field $V(r)$ which is the same for all the individual nucleons, like the Thomas-Fermi field for an atom. Such a field does not exist in the rigorous sense of the theory of Fock, but must be identified with some sort of average of the $\mathcal{W}_\nu(r)$ in (52) over all the occupied states R_0, R_1, R_2, etc. One way of introducing an approximate central field, denoted by $\mathcal{W}_\nu'(r)$ for a neutron and $\mathcal{W}_\pi'(r)$, for a proton, is to follow the idea of Slater[13] of using a weighted exchange potential suggested for the problem of an electron in an atom or in a metal. It is to be remembered that, apart from the fact that the $\mathcal{W}'(r)$ so defined is only approximate, $\mathcal{W}'(r)$ serves only as a convenient help to visualize the "central field" approximation and is not essential in the theory, since the binding energy of a nucleon in any shell can be obtained directly from the difference between the total energies of the two nuclei having A and $A-1$ nucleons. For this reason, we shall not overemphasize the significance of any such average central field, but give the potential $W(r)$ in (53) and similar equations for the $(1p)_N$, $(1s)_P$, and $(1p)_P$ in the O^{16} nucleus. For our present illustrative purpose, we have chosen $a_W'=\frac{1}{3}$ in (33) and $(\alpha+\beta)=-5b/3$ in (48), and have made the same approximation as in (46ν) and (46π). The result is shown in Fig. 1.[14]

[13] J. C. Slater, Phys. Rev. **81**, 385 (1951).

TABLE III. Binding energy of last particle in O^{16} and O^{15}.

Nucleus	O^{16}	O^{15}
Kinetic energy	23.50[a]	23.50
Potential energy	−69.79	−65.76
$(1s)_N$: λ_0	−46.29	−42.26
Coulomb energy	5.56	3.99
$(1s)_P$: ϵ_0	−40.73	−39.27
Kinetic energy	41.40	41.40
Potential energy	−45.26	−41.07
$(1p)_N$: λ_1	−3.86	0.33
Coulomb energy	5.20	2.53
$(1p)_P$: ϵ_1	1.34	2.86

[a] All energies are given in Mev.

It is also of interest to obtain the "central field" for the nucleons by further simplifying the Fock system (46) by making the Hartree approximation. This is done by neglecting all the "exchange" terms from the Fock equations (41), (42). We shall denote this "Hartree" field by $\mathcal{U}(r)$. Thus instead of (46ν), (46π), for example, we consider

$$[H_0+\mathcal{U}_\nu(r)-\lambda_0]R_0(r)=0, \tag{54}$$
$$[H_0+\mathcal{U}_\pi(r)-\epsilon_0]S_0(r)=0, \tag{55}$$

where

$$\mathcal{U}_\nu(r)=V_\nu(r)-(\alpha+\beta)V_{\nu\nu}{}^0(0,0;r),$$
$$\mathcal{U}_\pi(r)=V_\pi(r)-(\alpha+\beta)V_{\pi\pi}{}^0(0,0;r)-U^0(0,0;r). \tag{56}$$

Again, with $a_d=0$ and $(\alpha+\beta)=-5b/3$ in (48), one obtains the following "effective central field" for the $1s$, $1p$ neutron and protons in O^{16} in the Hartree approximation:

$$(1s)_N:\quad \mathcal{U}_\nu(r)=(5/3)bV_{\nu\nu}{}^0(0,0;r),$$
$$(1s)_P:\quad \mathcal{U}_\pi(r)=(5/3)bV_{\pi\pi}{}^0(0,0;r)+U^0(0,0;r)+6U^0(1,1;r),$$
$$(1p)_N:\quad \mathcal{U}_\nu(r)=(5/3)b[V_{\nu\nu}{}^0(1,1;r)+\tfrac{2}{5}V_{\nu\nu}{}^2(1,1;r)],$$
$$(1p)_P:\quad \mathcal{U}_\pi(r)=(5/3)b[V_{\pi\pi}{}^0(1,1;r)+\tfrac{2}{5}V_{\pi\pi}{}^2(1,1;r)]+2U^0(0,0;r)+5U^0(1,1;r)-\tfrac{2}{5}U^2(1,1;r). \tag{57}$$

[14] Recently P. Gombas [Acta Phys. Acad. Sci. Hung. **5**, 511 (1956)], in a treatment based on the Thomas-Fermi statistical model, has obtained potentials of shapes similar to those in Fig. 1.

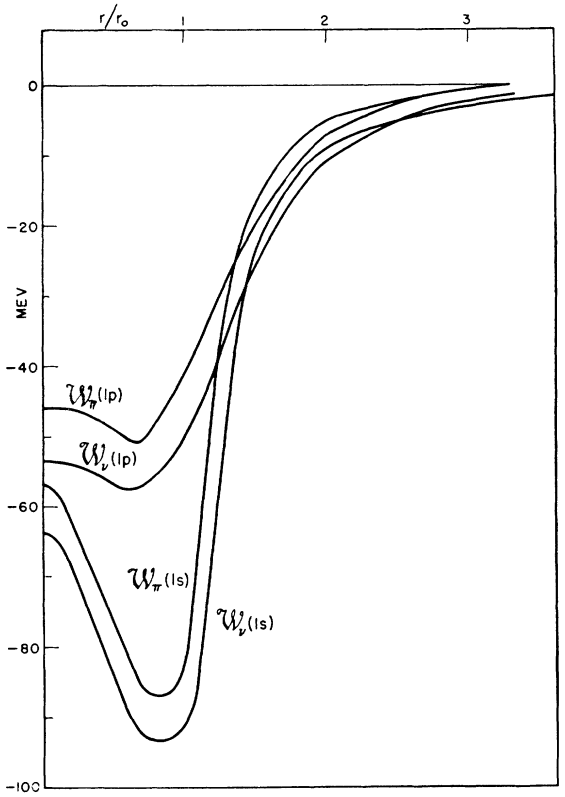

FIG. 1. Central field in the Fock approximation for $1s$, $1p$ neutron and proton in O^{16} nucleus. r_0 is the parameter in (10) and $\mathcal{W}(r)$ is given by (53) and similar expressions.

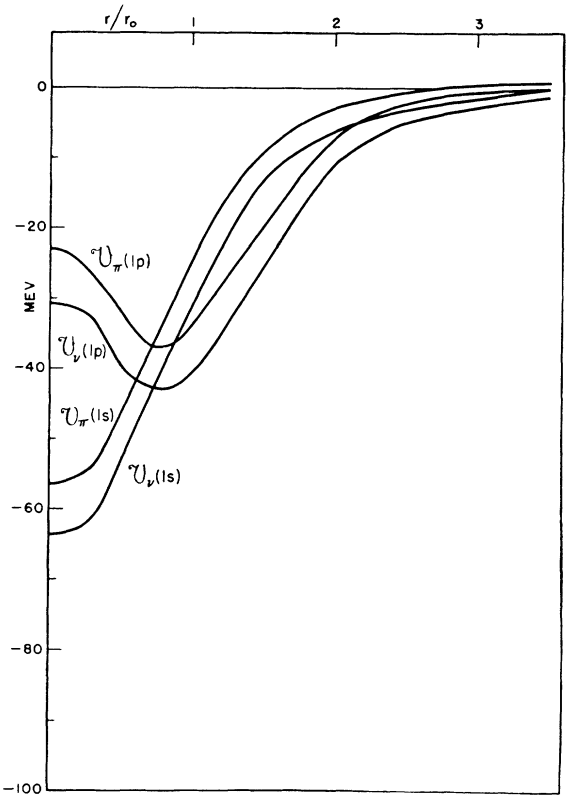

FIG. 2. Central field in the Hartree approximation for $1s$, $1p$ neutron and proton in O^{16} nucleus. r_0 is the parameter in (10) and $\mathcal{U}(r)$ is given by (57).

These central fields $\mathcal{U}_\nu(1s)$, $\mathcal{U}_\pi(1s)$, $\mathcal{U}_\nu(1p)$, and $\mathcal{U}_\pi(1p)$ are given in Fig. 2.

A comparison between these Hartree approximations and the Fock approximation $\mathcal{W}_\nu(r)$, $\mathcal{W}_\pi(r)$ shows that for any given "orbital," they differ considerably from each other; that the Fock fields $\mathcal{W}(r)$ are lower than the corresponding Hartree field $\mathcal{U}(r)$. It is also seen that, while the diffusive nature of the boundary of the fields is as expected [i.e., they reflect on the general nature of the wave function (18) employed], the Fock fields $\mathcal{W}_\nu(1s)$, $\mathcal{W}_\pi(1s)$, $\mathcal{W}_\nu(1p)$, and $\mathcal{W}_\pi(1p)$ all exhibit the interesting "wine-bottle" shape. It may be recalled that this wine bottle shape was introduced empirically before the advent of the spin-orbit coupling theory to account for the order of the nuclear energy levels and hence the magic-number nuclei. Thus it is interesting that this feature comes about without any additional assumption from the self-consistent (i.e., Fock's theory) treatment of the central-field approximation,[14] although one may not yet dispense with the assumption of a spin-orbit interaction to account for the magic-number nuclei. Further investigations of a few more nuclei in the neighborhood of the magic-number nuclei along the same line as described in the present paper are being carried out to throw more light on this point.

At this point, it is important to emphasize the difference between the $\mathcal{U}(r)$ in the Hartree approximation and the $\mathcal{W}(r)$ in the Fock approximation. One sees from (44), (45), (48), (56) that for sufficiently large negative values of a_d (i.e., $a_W' < \frac{1}{3}$), the $\mathcal{U}_\nu(r)$ and $\mathcal{U}_\pi(r)$ can become repulsive so that the individual nucleons are not bound to the rest of the nucleus at all. This result is of course inconsistent with the result in Table I which shows that the empirical binding energy of the nucleus is compatible with large negative values of a_d. This difference in the conclusion between the Hartree and the Fock approximation lies of course in the neglect of the "exchange" terms from the Fock equations (41) and (42), which are really very important in contributing to the binding of the nucleons. This illustrates the great difference between the central-field approximations in the atomic and the nuclear problem. In the atomic problem, the binding of the electrons and the "central field" comes primarily from the Coulomb field of the nucleus, and the Hartree approximation gives a fairly good approximation compared with the Fock approximation. In the nuclear problem, where there is no predominantly attractive central field, the "direct" and the "exchange" interactions between the nucleons are equally important and the neglect of the exchange terms in the Hartree ap-

proximation is a far more serious, in fact invalidating, approximation than in the case of the atomic problem.

The writers wish to thank Mr. R. Alford for helping with the calculations.

APPENDIX: EVALUATION OF THE INTEGRALS $V^k(n,m;r_i)$ AND $U^k(n,m;r_i)$

In order to evaluate the integrals defined by (38) and (39), the following method has proved useful. If one uses the integral representation for w_k [Eq. (22)], a typical one of the above integrals becomes

$$V^k(m,n;r_i)=\frac{2k+1}{2}\int\int\int R_m(r_j)R_n(r_j)\times J(r_{ij})P_k(\cos\Theta)d\cos\Theta dr_j, \quad \text{(A-1)}$$

where Θ is the angle between $\mathbf{r}_i$ and $\mathbf{r}_j$. Integration is to be carried out over the space of particle j, and for that purpose it is sufficient to choose $\mathbf{r}_i$ as the polar axis. If we now define new coordinates r and ψ by

$$r_i-r_j\cos\Theta=r\cos\psi, \quad r_j\sin\Theta=r\sin\psi, \quad \text{(A-2)}$$

the volume element $r_j^2dr_jd\cos\Theta$ transforms into $r^2drd\cos\psi$ and integration over r_j can be replaced by that over r. The integration over the angle ψ can be readily carried out in terms of the following integrals

$$I(\alpha,b)=\int_{-1}^{1}e^{\alpha x}x^b dx=e^{\alpha}\sum(-1)^m\frac{S_m{}^b}{\alpha^{m+1}}-e^{-\alpha}\sum\frac{S_m{}^b}{\alpha^{m+1}}, \quad \text{(A-3)}$$

where

$$x=\cos\psi, \quad \alpha=2rr_i\nu, \quad S_0{}^b=1,$$
$$S_m{}^b=b(b-1)\cdots(b-m+1), \quad m\neq 0,$$

while integrations over r results in integrals of the type

$$\zeta_l{}^{\pm}=\int_0^{\infty}\exp[-\nu(r_i{}^2+r^2)]\exp(\pm 2rr_i\nu)J(r)r^l dr, \quad \text{(A-4)}$$

whose evaluation leads to error functions.

The evaluation of the U integrals proceeds similarly, except that (A-4) is now replaced by the simpler expression

$$\eta_l{}^{\pm}=e^2\int_0^{\infty}\exp[-\nu(r_i{}^2+r^2)]\exp(\pm 2rr_i\nu)r^{l-1}dr. \quad \text{(A-5)}$$

For the integrals occurring in (38)–(57), one obtains finally the following expressions:

$$V^0(0,0;r_i)=\frac{\lambda V_0}{2\rho}\exp(-\rho^2)[f_{\pm}(\sigma)-f(\tau)],$$

$$V^1(0,1;r_i)=\left(\frac{3}{2}\right)^{\frac{1}{2}}\frac{\lambda V_0}{2\rho}\exp(-\rho^2)\left[-\frac{4}{\sqrt{\pi}}\rho+f_{\pm}(\sigma)(2\rho^2+2\rho\sigma+1)-f(\tau)(2\rho^2-2\rho\sigma+1)\right],$$

$$V^0(1,1;r_i)=\frac{\lambda V_0}{6\rho}\exp(-\rho^2)\left[-\frac{4}{\sqrt{\pi}}\rho+(2\mu^2+3)[f_{\pm}(\sigma)-f(\tau)]\right], \quad \text{(A-6)}$$

$$V(1,1;r_i)\equiv V^0(1,1;r_i)+\tfrac{2}{5}V^2(1,1;r_i)$$
$$=\frac{\lambda V_0}{2\rho^3}\exp(-\rho^2)\left\{-\frac{4}{\sqrt{\pi}}(1+\rho^2)\rho+f_{\pm}(\sigma)[(2\rho^2+1)(\rho^2+1)+2\rho\sigma(2\rho^2+\rho\sigma+1)]-f(\tau)[(2\rho^2+1)(\rho^2+1)-2\rho\tau(2\rho^2-\rho\tau+1)]\right\},$$

where

$$f(\tau)=\exp(\tau^2)[1-\Phi(\tau)], \quad \tau=\mu+\rho,$$
$$f_{\pm}(\sigma)=\exp(\sigma^2)[1\pm\Phi(|\sigma|)] \text{ for } \rho>\mu \text{ or } \rho<\mu, \ \sigma=\mu-\rho,$$
$$\Phi(\rho)=\frac{2}{\sqrt{\pi}}\int_0^{\rho}\exp(-t^2)dt,$$
$$\rho=\nu^{\frac{1}{2}}r_i, \quad \lambda=\nu^{\frac{1}{2}}r_0, \quad \mu=1/2\lambda,$$

and

$$U^0(0,0;r)=\frac{e^2\nu^{\frac{1}{2}}}{\rho}\Phi(\rho),$$

$$U^1(0,1;r)=e^2\nu^{\frac{1}{2}}\left[\frac{1}{\rho^2}\Phi(\rho)-\frac{2}{\pi^{\frac{1}{2}}\rho}\exp(-\rho^2)\right],$$

$$U^0(1,1;r)=e^2\nu^{\frac{1}{2}}\left[\frac{1}{\rho}\Phi(\rho)-\frac{2}{3\sqrt{\pi}}\exp(-\rho^2)\right], \quad \text{(A-7)}$$

$$U(1,1;r)\equiv U^0(1,1;r)+\tfrac{2}{5}U^2(1,1;r)$$
$$=e^2\nu^{\frac{1}{2}}\left[\frac{1}{\rho^3}(\rho^2+1)\Phi(\rho)-\frac{2}{\pi^{\frac{1}{2}}\rho^2}(\rho+1)\exp(-\rho^2)\right].$$