

Properties of Finite Nuclei

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The application of the reaction-matrix theory to the calculation of binding energies and other properties of finite nuclei is investigated. We consider O^{16} and Ca^{40} . The single-particle wave functions are obtained from a self-consistent shell-model potential defined so as to minimize the total energy of the nucleus. The attractive part of the reaction matrix is derived from the long-range part of a central spin-independent potential acting in S states only. We treat the nonlocality of this reaction matrix in the effective-mass approximation and the nonlocal shell-model potential is then also obtained in the similar form. For the repulsive part of the reaction matrix we compare the local-density approximation of Brueckner and co-workers with a more detailed one. We find that the local-density approximation gives an underestimate of the binding by 2–2.5 MeV/nucleon. The center-of-mass correction increases the calculated binding further with 0.8 and 0.2 MeV/nucleon in O^{16} and Ca^{40} , respectively. We investigate the possibility of replacing the nonlocal shell-model potential by certain local potentials. We try the harmonic oscillator and the Gaussian potentials, minimizing the energy with respect to the one parameter for the first, and the two parameters for the second. The binding differs by not more than 0.2 MeV/nucleon between these local potentials and the nonlocal self-consistent potential. In fact the local potentials often give more binding, owing to approximations necessary in the self-consistent potential in some cases.

I. INTRODUCTION

IN a previous publication¹ we presented a formal theory of finite nuclei. The reaction-matrix (K -matrix) theory of nuclei has been applied rather extensively to the system of infinite nuclear matter.^{2–5} A main correlation between the nucleons can be included in the K matrix by suitable definition of this quantity. It was until rather recently believed that the energy of infinite nuclear matter could be calculated to a good approximation in first order of this K matrix as customarily defined.² However, recent results of Bethe⁶ show that higher order K -matrix terms (3-body terms) contribute several MeV. Thus in the future development of the theory, either one has to calculate these higher order terms explicitly, or one might manage to redefine the K matrix so as to include in it the important 3-body correlations previously omitted by its definition.

In I, we developed a scheme for applying the K -matrix theory to the finite nucleus. The K -matrix theory does not define the quantum-mechanical state of the system but provides in general only a means of calculating the total energy of the system in powers of a K matrix for a given state. In calculations on infinite nuclear matter, the state of the system specified, e.g., by the density, is usually obtained by searching for the minimum of total energy. In analogy with this procedure we defined for calculations on finite nuclei a shell-model potential so that the total energy is minimized. This defines the ground state of the nucleus by specifying

the wave functions as solutions of the Schrödinger equation with this shell-model potential.

The K matrix is a function of the state of the medium. It is quite a complicated numerical task to compute the K matrix in infinite nuclear matter, and far more complicated in a general finite system. Therefore one is forced to find an approximate method to calculate the K matrix in a finite medium. In I we concluded that not only the short-range but also the long-range part of the K matrix in configuration space would have to be treated as medium-dependent. Our conclusions were made from calculations of the rearrangement contributions to single-particle energies. In the calculations of Brueckner and co-workers only the core part was treated as density-dependent.^{7,8} In I as well as earlier⁹ we pointed out that the core term contains an important part which does not depend on a local (center-of-mass) density,^{10,11} but is proportional to the sum of the potential K -matrix energies of the two interacting nucleons. Thus the core term depends rather on some average density than on the center-of-mass density. We have also pointed out that this characteristic of the K matrix gives more binding for finite nuclei than if calculated by a local-density approximation.^{1,9}

However, the K matrix enters in a complicated way into the calculation of both the energy and the wave functions, determined by the shell-model potential. Therefore one has to investigate this point by actual calculations even to estimate the corrections.

It is an object of primary interest in this paper to investigate the effect on binding energy and density

¹ H. S. Köhler, Phys. Rev. **137**, B1145 (1965) (referred to as I).

² K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).

³ S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) **11**, 65 (1960).

⁴ H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963).

⁵ K. A. Brueckner and K. S. Masterson, Jr., Phys. Rev. **128**, 2267 (1962).

⁶ H. A. Bethe (to be published).

⁷ K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961) (referred to as BLR).

⁸ K. S. Masterson, Jr., and A. M. Lockett, Phys. Rev. **129**, 776 (1963).

⁹ H. S. Köhler, Nucl. Phys. **38**, 661 (1962).

¹⁰ K. A. Brueckner, J. L. Gammel, and H. Weitzner, Phys. Rev. **110**, 431 (1958).

¹¹ K. A. Brueckner, and D. T. Goldman, Phys. Rev. **116**, 424 (1959).

distributions by replacing the K matrix calculated by a local-density approximation with one more detailed, as previously described.^{1,9}

The shell-model potential obtained is nonlocal. In order to speed up the calculations and make possible more extensive calculations, we expanded to second order in the nonlocality. Thereby the problem of calculating the wave functions was considerably simplified. In general, this will involve the solution of an integrodifferential equation, since the potential is nonlocal. The expansion reduces this to a second-order differential equation similar to a customary Schrödinger equation, although a first-order derivative term now also appears.

The definition of a shell-model potential, as in I, that gives wave functions that minimize the total energy means, in principle, a variation with respect to an infinite number of parameters. It is of practical interest to know how important the exact definition of the shell-model potential is. Thus we may choose a potential which is a function of only a few parameters like surface thickness, depths, etc., and vary these parameters so as to minimize the energy. Of course, we do not thereby reach the absolute minimum, but only a minimum within the class of states defined by the special choice of parametrical expression for the potential that we choose. We find in this paper that for calculations of the binding of O^{16} and Ca^{40} both the harmonic oscillator and the Gaussian potentials are quite adequate.

II. CHOICE OF NUCLEON-NUCLEON INTERACTION

Our aim in this paper is not to start with some "exact" nucleon potential and with this try to reproduce known bindings, etc., by applying the K -matrix theory. This was tried before.^{7,8} However, on that occasion an approximate medium dependence for the K matrix was used: the local density approximation. We have tried to improve on this approximation.^{1,9} It is of immediate interest to investigate if this would appreciably improve the results for binding energy, etc. We also wish to make other tests and checks on possible approximation procedures so that a calculation on a finite nucleus can be made practically with sufficient accuracy.

The shell-model potential is in general nonlocal. Therefore we have to solve an integrodifferential equation to obtain the single-particle wave functions. This is, however, quite time consuming on the computer.⁸ The Schrödinger equation will contain a term $\int \mathcal{U}(\mathbf{r}, \mathbf{r}') \times \psi(\mathbf{r}') d\mathbf{r}'$ where \mathcal{U} is the shell-model potential and ψ a single-particle wave function. However, we can expand in powers of the momentum conjugate to $\mathbf{r} - \mathbf{r}'$ and if we keep only terms up to some order $n \geq 2$ the integrodifferential equation will be reduced to a differential equation of order n . If we thus expand to second order only, the equation will be of the order of a customary second-order wave equation. This procedure is referred to as an effective-mass approximation; a term similar

to the kinetic-energy term will appear and can be included in this by defining an effective mass.

The shell-model potential is derived from the K matrix. Rather than approximate on the shell-model potential, we therefore preferred to approximate on the K matrix in such a way that the shell-model potential derived from it gives an effective-mass approximation as defined above.

We further decided to deal only with S -state interactions. This is, as discussed in previous publications, the most important part of the interaction in nuclear matter, and also carries most of the medium dependence. We have further neglected spin dependence. The spin-orbit force giving rise to the spin-orbit splittings is, as is now well known, important for the explanation of the nuclear shell structure. Also we expect the tensor force to be important for the binding, as it has been found to be in infinite nuclear matter. However, we omit these details of the nucleon interaction in this investigation.

We shall thus deal only with a central, spin-independent, S -state nucleon interaction. We split the K matrix into parts and, as discussed in I, a main part, the long-range part, is static, i.e., independent of the structure of the medium. Of the medium-dependent parts discussed in I we shall here, as mentioned in the Introduction, be concerned only with the short-ranged repulsive part. The static part is attractive. We shall call it K_a . We shall then achieve our goal of an effective-mass approximation by assuming it to have a form

$$(\mathbf{r} | K_a | \mathbf{r}') = \alpha v_0(r) \delta(\mathbf{x}) + \beta v_2(r) (\mathbf{e}_r \times \nabla)^2 \delta(\mathbf{x}), \quad (1)$$

where \mathbf{e}_r is the unit vector along \mathbf{r} , and

$$\mathbf{x} = \mathbf{r} - \mathbf{r}'. \quad (1a)$$

The $\mathbf{e}_r \times \nabla$ term is explained later. In momentum space thus

$$(\mathbf{k}'' | K_a | \mathbf{k}') = \alpha \bar{v}_0(q) + \beta k^2 \bar{v}_2(q), \quad (2)$$

where $\mathbf{k} = \frac{1}{2}(\mathbf{k}'' + \mathbf{k}')$, $\mathbf{q} = \mathbf{k}'' - \mathbf{k}'$, and

$$\bar{v}_0(q) = \int e^{i\mathbf{q} \cdot \mathbf{r}} v_0(r) d\mathbf{r}, \quad (2a)$$

$$\bar{v}_2(q) = \int e^{i\mathbf{q} \cdot \mathbf{r}} v_2(r) \sin^2 \alpha d\mathbf{r}.$$

α is the angle between \mathbf{k} and \mathbf{e}_r . Diagonal elements in momentum space will thus be

$$(\mathbf{k} | K_a | \mathbf{k}) = a + bk^2, \quad (3)$$

where

$$a = \alpha \bar{v}_0(0) \quad \text{and} \quad b = \beta \bar{v}_2(0).$$

In all our calculations we treated α and β as parameters, adjusting them so that the K_a matrix of (3), together with the repulsive core term to be discussed later, gives saturation of the infinite system at a specified density and binding energy.

We further have to choose the functions $v_0(r)$ and $v_2(r)$. In some preliminary test calculations, some of which we shall present, we just used δ functions. It is clear however that both v_0 and v_2 must have the range of the nucleon force. It would probably be sufficient to use an exponential or similar function of the appropriate range. In order to relate v_0 and v_2 more strongly to some realistic nucleon force, we assumed K_a to be given by the long-range part of the Moszkowski-Scott potential interacting in S states.³ Thus

$$\langle \mathbf{r} | K_a | \mathbf{r}' \rangle = v(r) \delta(r-r') / 4\pi r^2, \quad (4)$$

where

$$\begin{aligned} v(r) &= V_0 e^{-\mu r}, & r > d \\ v(r) &= 0, & r < d \end{aligned} \quad (4a)$$

with $V_0 = -603.06$ MeV, $\mu = 2.083$ F⁻¹, $d = 1.1$ F. By means of the δ function we include only s -state interactions. We expand (4) in the momentum conjugate to nonlocality coordinate \mathbf{x} . Thus

$$\begin{aligned} \langle \mathbf{r} | K_a | \mathbf{r}' \rangle &= \left\{ \int v(r) \delta(r-r') \left[1 + \mathbf{x} \cdot \nabla + \frac{1}{2} (\mathbf{x} \cdot \nabla)^2 \right] d\mathbf{x} \right\} \\ &\quad \times \delta(\mathbf{x}) / 4\pi r^2, \end{aligned} \quad (5)$$

which is perhaps an unusual way to write a Taylor expansion, but quite straightforward with the use of δ functions. The gradients operate on $\delta(\mathbf{x})$. With (4a) the first integral (\mathcal{J}_0) gives

$$\mathcal{J}_0 = \frac{V_0}{4\pi} \int \frac{e^{-\mu r}}{r^2} \delta[r - (4r_1^2 + r^2 - 4rr_1 \cos\theta)^{1/2}] 8dr, \quad (6)$$

where $\mathbf{r}_1 = \frac{1}{2}(\mathbf{r} + \mathbf{r}')$; thus $\mathbf{x} = 2\mathbf{r}_1 - 2\mathbf{r}$ and θ is the angle between \mathbf{r} and \mathbf{r}_1 . We do the angular integration by putting $\cos\theta = t$, $z^2 = 4r_1^2 + r^2 - 4rr_1 t$ and

$$\mathcal{J}_0 = \frac{2V_0}{r_1} \int e^{-\mu r} dr. \quad (7)$$

From (4a) we get the conditions $r_1 > d$, $r > r_1$ and $r_1 < d$, $r > d$. Thus

$$\mathcal{J}_0 = (2V_0/\mu r) e^{-\mu y}, \quad (8)$$

with

$$y = d \text{ for } r < d, \quad y = r \text{ for } r > d. \quad (9)$$

The two remaining integrals are performed similarly. Owing to the spherical symmetry (filled-shell nuclei) of the nuclear systems to be studied, the term with one gradient averages to zero when computing a matrix element of K_a . Thus we can write

$$\langle \mathbf{r} | K_a | \mathbf{r}' \rangle = v_0(r) \delta(\mathbf{x}) + v_2(r) (\mathbf{e}_r \cdot \nabla)^2 \delta(\mathbf{x}), \quad (10)$$

with

$$\begin{aligned} v_0(r) &= (2V_0/\mu r) e^{-\mu y}, \\ v_2(r) &= \frac{2V_0}{r^3} e^{-\mu y} \left(\frac{y^2}{\mu} + \frac{2y}{\mu^2} + \frac{2}{\mu^3} - \frac{r^2}{\mu} \right), \end{aligned} \quad (10a)$$

with y given by (9).

In (10) the $\mathbf{e}_r \cdot \nabla$ term appears because the non-locality of the central s -state interaction is only along coordinates perpendicular to \mathbf{r} , while along \mathbf{r} the interaction is local because of the $\delta(r-r')$ factor in (4).

We now let the functions $v_0(r)$ and $v_2(r)$ in (1) be determined by (10a). With $\alpha = 1$ and $\beta = 1$ one gets in (3) $a = -1005.6$ MeV F³ and $b = 1420.2$ MeV F⁵. In order that the assumption of the force (4) and the expansion (5) shall make sense, our parameters α and β , when adjusted to give correct saturation, should of course not deviate too much from the value 1. In fact we shall find $\alpha \approx 1$ and $\beta \approx 0.4$. The smaller value of β is because in the exact expression of K in \mathbf{k} and \mathbf{q} (2) the function of \mathbf{k} is more like a Gaussian than a parabola. The second-order expansion in \mathbf{k} is not strictly good, and the error has to be compensated by a small β . However, we still think the functions (10a) are sufficiently realistic.

For the repulsive part of the K matrix we have as a main object of this investigation compared the local density approximation^{7,8,10,11} with the one described in I. We have also here chosen to use parametric expressions so as always to be able to "normalize" the interactions to equal saturations of the infinite nuclear system. How this is done exactly is described later. The core term of the local density approximation as given in Ref. 11 is nonvanishing for zero density. However, by using for the attractive part K_a a potential that vanishes for $r < d$ (4) we have in fact included in the core term the attraction for $r < d$ in such a way that the repulsive term should vanish at zero density.^{3,12}

Brueckner and Goldman¹¹ put for their core term

$$\langle \mathbf{r} | K(\rho) | \mathbf{r}' \rangle = A(\rho) \delta(r-c) \delta(r'-c) / 4\pi c^2, \quad (11)$$

where c is the core radius and

$$A(\rho) = r_1 / (1 - \delta \rho^{1/3}), \quad (11a)$$

in which γ_1 and δ are parameters (depending on spin state) which are adjusted so that (11) gives the calculated repulsion in an infinite system. ρ is the density. As mentioned above, we are interested in the repulsion K^I obtained by subtracting from (11) the zero-density value. Thus we shall use

$$\langle \mathbf{r} | K^I(\rho) | \mathbf{r}' \rangle = [\gamma \rho^{1/3} / (1 - \delta \rho^{1/3})] \delta(\mathbf{r}) \delta(\mathbf{r}'), \quad (11b)$$

with $\gamma = \gamma_1 \times \delta \times 4\pi c^2$. In (11b) we have further replaced $\delta(r-c)$ by $\delta(r)$, since the core radius is very small relative to nucleon wavelengths ($k_F c \ll 1$). From Ref. 11 we get

$$\begin{aligned} \text{singlet: } & \delta = 0.787 \text{ F}, \quad \gamma = 185.0 \text{ MeV F}^3, \\ \text{triplet: } & \delta = 0.740 \text{ F}, \quad \gamma = 218.8 \text{ MeV F}^3. \end{aligned} \quad (11c)$$

As we use the spin-independent interaction, we average to

$$\delta = 0.763 \text{ F}, \quad \gamma = 202.6 \text{ MeV F}^3. \quad (11d)$$

¹² H. S. Köhler, Ann. Phys. (N. Y.) 16, 375 (1961).

In I (Eqs. 27, 29) and in Ref. 9 we derived a K -matrix repulsion, which we shall call K^{II} as distinguished from K^{I} of (11).

$$K_{ij,ij}^{\text{II}} = - \int \chi^2(\mathbf{r}) d\mathbf{r} \int \rho_i(\mathbf{R}) \rho_j(\mathbf{R}) d\mathbf{R} (V_i + V_j) \\ + 2 \int \rho_i(\mathbf{R}) \rho_j(\mathbf{R}) \chi^2(k) V(k, \rho(\mathbf{R})) d\mathbf{R} d\mathbf{k}. \quad (12)$$

Here χ is a two-particle correlation as described in I, and V is the K -matrix potential energy of the specified state. We assume that the excited-state potential energy in (12) is given by⁴ $V(k, \rho(R)) = \text{const} \rho(R) k^2$. The integration over momentum \mathbf{k} in (12) depends on the details of χ , and we assume it to give

$$2 \int \chi^2(k) V(k, \rho(R)) d\mathbf{k} = c_2 \rho(R). \quad (13)$$

Unfortunately c_2 can only be roughly estimated to be

$$c_2 = 150 \text{ MeV F}^3. \quad (13a)$$

The core-correlation volume we call c_1 . Thus

$$c_1 = \int \chi^2(\mathbf{r}) d\mathbf{r} \quad (14)$$

and we have previously^{1,9,13} calculated $c_1 = 0.5$ to 1.0. We can now write a parametrical expression for the repulsion K^{II} in coordinate space as

$$\langle \mathbf{r}_1 \mathbf{r}_2 | K^{\text{II}} | \mathbf{r}_1' \mathbf{r}_2' \rangle \\ = -c_1 [\langle \mathbf{r}_1 | V | \mathbf{r}_1' \rangle + \langle \mathbf{r}_2 | V | \mathbf{r}_2' \rangle] \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1' - \mathbf{r}_2') \\ + c_2 \rho(R) \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1' - \mathbf{r}_2'), \quad (15)$$

where the potential energy operators V are obtained from

$$\langle \mathbf{r} | V | \mathbf{r}' \rangle = \sum_{\mathbf{k}} \int \varphi_{\mathbf{k}}(\mathbf{r}_1) \langle \mathbf{r}_1 \mathbf{r} | K | \mathbf{r}_1' \mathbf{r}' \rangle \\ \times \varphi_{\mathbf{k}}(\mathbf{r}_1') d\mathbf{r}_1 d\mathbf{r}_1' - \text{exch}, \quad (15a)$$

where $\varphi_{\mathbf{k}}$ are the single hole states. As explained in I, the matrix K^{II} of (15) corresponds to third-order K -matrix graphs—the first term to hole-bubble and the second to particle-bubble graphs. Momentum conservation does *not* prevent nondiagonal hole or particle states, as the states φ are not eigenfunctions of momenta for finite systems. However, we shall not include these nondiagonal graphs, which should only give small corrections. We leave the study of them to a later investigation. Therefore the prescription is now to include in (15) only diagonal elements of V with respect to φ . Further, in (15) the δ functions represent the short-range core correlation: the first and last interactions of the third-order graphs.

¹³ J. Dabrowski and H. S. Köhler, Phys. Rev. **136**, B162 (1964).

Most of the calculations presented in this paper are made with the attractive part of the K matrix of Eq. (1) where $v_0(\mathbf{r})$ and $v_2(\mathbf{r})$ either are δ functions or are given by (10a). The repulsive part is given either by the local density approximation K^{I} (11c) or by the more exact expression K^{II} (15). The parameters of these interactions are determined as will now be described.

III. DETERMINATION OF PARAMETERS FROM INFINITE MEDIUM CALCULATIONS

The parameters are determined by an adjustment of the infinite nuclear matter system to known data. The binding energy and saturation density are given experimentally.

With K_a given by (3) we obtain the contribution V_a for the K -matrix energy from the attractive interaction,

$$V_a(k_1) = - \frac{3}{4} \frac{4}{(2\pi)^3} \int_0^{k_F} e^{-i\mathbf{k}_1 \cdot \mathbf{r}_1 - i\mathbf{k}_2 \cdot \mathbf{r}_2} (a + bk^2) e^{i\mathbf{k}_1 \cdot \mathbf{r}_1 + i\mathbf{k}_2 \cdot \mathbf{r}_2} d\mathbf{k}_2, \quad (16)$$

where $\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$ is the relative momentum and k_F the Fermi momentum. The factor $\frac{3}{4}$ comes from the spin statistics for a S -state interaction in a filled-shell nucleus¹⁴ and therefore appears throughout this paper. Note that the exchange term is included in (16) by this factor. After the integration in (16) and with the density ρ given by

$$\rho = 2k_F^3/3\pi^2, \quad (17)$$

we get

$$V_a(k) = \frac{3}{4} a \rho + \frac{9b}{80} \left(\frac{3\pi^2}{2} \right)^{2/3} \rho^{5/3} + \frac{3b}{16} \rho k^2. \quad (16a)$$

As expected, this is of the form of the effective-mass approximation. Further, the contribution from K_a for the potential energy per particle, P_a , is

$$P_a = \frac{1}{2} \int_0^{k_F} V_a(k) d\mathbf{k} / \int_0^{k_F} d\mathbf{k} \quad (18)$$

or

$$P_a = \frac{3}{8} a \rho + \frac{9b}{80} \left(\frac{3\pi^2}{2} \right)^{2/3} \rho^{5/3}. \quad (18a)$$

Further, the repulsive term K^{I} (11b) gives similarly $V^{\text{I}}(k_1)$, which is independent of k_1 , i.e.,

$$V^{\text{I}} = \frac{3}{4} \gamma \rho^{4/3} / (1 - \delta \rho^{1/3}) \quad (19)$$

and

$$P^{\text{I}} = \frac{3}{8} \gamma \rho^{4/3} / (1 - \delta \rho^{1/3}). \quad (20)$$

As the K^{I} matrix depends on density, it gives rise to a rearrangement contribution to the energy of real holes. This can be calculated as by Brueckner and Goldman¹¹ or we can use the Hugenholtz-van Hove

¹⁴ H. A. Bethe, Phys. Rev. **103**, 1353 (1956).

theorem,¹⁵ which we write as

$$\mathcal{E}(k_F) = E/A + \rho(d/d\rho)(E/A), \quad (21)$$

where E/A is the energy per particle and $\mathcal{E}(k_F)$ the energy of a real hole at the Fermi surface, i.e.,

$$\mathcal{E}(k) = V(k) + V_R(k) + T(k), \quad (21a)$$

where T is the kinetic energy. Now (21) is satisfied when calculating contributions to E/A and \mathcal{E} from the kinetic energy operator and from K_a . We thus obtain immediately the rearrangement contribution to V from K^I . We call this quantity $V_R^I(k)$; it is independent of momentum k . Thus

$$V_R^I = P^I + \rho(d/d\rho)P^I - V^I \quad (22)$$

and we get

$$V_R^I = \frac{1}{8}\gamma\rho^{4/3}/(1-\delta\rho^{1/3})^2. \quad (23)$$

We further get from (15) in an infinite system

$$(\mathbf{k}_1\mathbf{k}_2|K^{II}|\mathbf{k}_1\mathbf{k}_2) = -c_1[V(k_1) + V(k_2)] + c_2\rho, \quad (24)$$

with unit volume of the box in which the plane waves are normalized. Here V is the first-order K -matrix energy. Thus

$$V(k) = V_a(k) + V^{II}(k) \quad (25)$$

and $V^{II}(k)$ is obtained from K^{II} by

$$V^{II}(k) = -\frac{3}{4}\frac{1}{(2\pi)^3}c_1\int_0^{k_F}[V(k) + V(k_2)]d\mathbf{k}_2 + \frac{3}{4}\frac{\rho}{(2\pi)^3}c_2\int_0^{k_F}d\mathbf{k}_2 \quad (26)$$

or

$$V^{II}(k) = -\frac{3}{4}c_1\rho[V(k) + 2P] + \frac{3}{4}c_2\rho^2, \quad (26a)$$

where P is the total potential energy. Thus

$$P = \frac{1}{2}\int_0^{k_F}V(k)d\mathbf{k}. \quad (27)$$

From (26a) we further obtain the potential energy per particle due to K^{II} ,

$$P^{II} = -\frac{3}{4}c_1\rho P + \frac{3}{8}c_2\rho^2. \quad (28)$$

Thus, also

$$P = P_a + P^{II} \quad (29)$$

so that with (28)

$$P = (P_a + \frac{3}{8}c_2\rho^2)/(1 + \frac{3}{4}c_1\rho). \quad (30)$$

The rearrangement potential $V_R^{II}(k)$ will now be a function of momentum k . We can again obtain $V_R^{II}(k_F)$ from the relations (21), (30), (16a), and (26a). Thus

$$V_R^{II}(k_F) = -\frac{3}{4}c_1\rho V(k_F)/(1 + \frac{3}{8}c_1\rho) + \frac{3}{8}c_2\rho^2(r). \quad (31)$$

This result is of some immediate interest. The expression (31) is in fact a rearrangement contribution for all orders in K . In I we calculated the lowest order con-

tribution to V_R from the K^{II} matrix, i.e., to third order in K . We then obtained the hole-bubble contribution

$$V_{R,h}^{II}(k) = -\frac{3}{4}c_1\rho V(k). \quad (32)$$

We thus find by comparison with the first term of (31) that at the Fermi surface the result (32) should be corrected by a factor $(1 + \frac{3}{8}c_1\rho)^{-1} = 0.87$ at $\rho = 0.2 \text{ F}^{-3}$ and with $c_1 = 0.5 \text{ F}^3$ (the factor is 0.77 for $c_1 = 1.0$). Thus the rearrangement potential is overestimated by some 10–20% at the Fermi momentum by only including the lowest order rearrangement term. We may expect a similar correction at other momenta.

To determine the parameters α and β when working with the interaction $K_a + K^I$, a saturation density $\rho_0 = 0.1948 \text{ F}^{-3}$ and a total energy per particle -15.5 MeV were assumed. At saturation the second term of the right-hand side of (21) is zero. Then

$$\mathcal{E}(k_F) = E/A \quad (33)$$

and

$$E/A = -15.5 \text{ MeV} \quad (34)$$

determines α and β . The quantities γ and δ are given by (11d), but we also calculated with some other values of γ and δ , while keeping P^I of (20) the same as with the values (11d).

When working with $K_a + K^{II}$ we have to determine the four parameters α , β , c_1 , and c_2 . We first assumed a value of c_2 for the particle-bubble interaction. Then α , β , and c_1 were determined using (33), (34) and putting $P^{II} = P^I$, where again P^I was obtained from (20) with γ and δ from (11d).

IV. FIRST-ORDER K -MATRIX ENERGIES

As discussed in I we now calculate the potential energies of the system to first order in K , as has been done for the treatment of the infinite system. Thus the potential energy is given by

$$P = \frac{1}{2} \times \frac{3}{4} \sum_{ij} \int \varphi_i^*(\mathbf{r}_1) \varphi_j^*(\mathbf{r}_2) (\mathbf{r}|K|\mathbf{r}') \varphi_i(\mathbf{r}_1') \varphi_j(\mathbf{r}_2') \times d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2', \quad (35)$$

where $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{r}' = \mathbf{r}_1' - \mathbf{r}_2'$ and the functions φ are the single-particle wave functions (of the ground state). As before, the exchange term is included by means of the factor $\frac{3}{4}$, as we are working with filled shells.

The single-particle potential energy V_i enters into the resolutive K^{II} matrix (12) and

$$V_i = \frac{3}{4} \sum_j \varphi_i^*(\mathbf{r}_1) \varphi_j^*(\mathbf{r}_2) (\mathbf{r}|K|\mathbf{r}') \varphi_i(\mathbf{r}_1') \varphi_j(\mathbf{r}_2') \times d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2'; \quad (36)$$

also, from (35),

$$P = \frac{1}{2} \sum_i V_i. \quad (35a)$$

In coordinate space we have from (15a)

$$(\mathbf{r}_1|V|\mathbf{r}_1') = \frac{3}{4} \sum_j \varphi_j(\mathbf{r}_2) (\mathbf{r}|K|\mathbf{r}') \varphi_j(\mathbf{r}_2') d\mathbf{r}_2 d\mathbf{r}_2', \quad (37)$$

¹⁵ N. M. Hugenholtz and L. van Hove, *Physica* **24**, 363 (1958).

often referred to as the Hartree-Fock potential because it is of first order in K . It is, as we shall find, the main contribution to the shell-model potential. We now let V operate on φ_i and calculate

$$(\mathbf{r}_1|V|\varphi_i) = \frac{3}{4} \sum_j \varphi_j(\mathbf{r}_2)(\mathbf{r}|K|\mathbf{r}') \varphi_j(\mathbf{r}_2') \varphi_i(\mathbf{r}_1') \times d\mathbf{r}_2 d\mathbf{r}_2' d\mathbf{r}_1'. \quad (38)$$

We can perform the integration over \mathbf{r}_2' using the implicit δ function on the center-of-mass coordinate. With the notation (1a) we get

$$(\mathbf{r}_1|V|\varphi_i) = \frac{3}{4} \sum_j \varphi_j(\mathbf{r}_1 - \mathbf{r})(\mathbf{r}|K|\mathbf{r} + \mathbf{x}) \times \varphi_j(\mathbf{r}_1 - \mathbf{r} + \frac{1}{2}\mathbf{x}) \varphi_i(\mathbf{r}_1 + \frac{1}{2}\mathbf{x}) d\mathbf{r} d\mathbf{x}. \quad (39)$$

We now insert K_a for K and get with (1)

$$(\mathbf{r}_1|V_a|\varphi_i) = \frac{3}{4} \sum_j \int [\alpha v_0(\mathbf{r})\delta(\mathbf{x}) + \beta v_2(\mathbf{r})(\mathbf{e}_r \cdot \nabla)^2 \delta(\mathbf{x})] \times \varphi_j(\mathbf{r}_1 - \mathbf{r}) \varphi_j(\mathbf{r}_1 - \mathbf{r} - \frac{1}{2}\mathbf{x}) \varphi_i(\mathbf{r}_1 + \frac{1}{2}\mathbf{x}) d\mathbf{r} d\mathbf{x}. \quad (40)$$

The first term on the right-hand side is readily evaluated. To evaluate the second we use the relation from the definition of a δ function

$$\int \nabla^2 \delta(x) F(x) dx = \left(\frac{d^2 F(x)}{dx^2} \right)_{x=0}. \quad (41)$$

We then get

$$(\mathbf{r}|V_a|\varphi_i) = V_a^{(0)}(\mathbf{r}) \varphi_i(\mathbf{r}) + V_a^{(1)}(\mathbf{r}) \mathbf{e}_r \cdot \nabla \varphi_i(\mathbf{r}) + V_a^{(2)}(\mathbf{r}) \nabla^2 \varphi_i(\mathbf{r}), \quad (42)$$

with

$$V_a^{(0)}(\mathbf{r}) = \frac{3}{4} \alpha \int v_0(r_1) \rho(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1 + \frac{3}{16} \beta \int v_2(r_1) \sin^2 \theta \rho_2(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1, \quad (42a)$$

$$V_a^{(1)}(\mathbf{r}) = \frac{3}{16} \beta \int v_2(r_1) \sin^2 \theta \mathbf{e}_{r_1} \cdot \nabla \rho(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1, \quad (42b)$$

$$V_a^{(2)}(\mathbf{r}) = \frac{3}{16} \beta \int v_2(r_1) \sin^2 \theta \rho(\mathbf{r} - \mathbf{r}_1) d\mathbf{r}_1. \quad (42c)$$

Here the angle θ is between \mathbf{r} and \mathbf{r}_1 . Further

$$\begin{aligned} \rho(\mathbf{r}) &= \sum_j \varphi_j^*(\mathbf{r}) \varphi_j(\mathbf{r}), \\ \rho_2(\mathbf{r}) &= \sum_j \varphi_j^*(\mathbf{r}) \nabla^2 \varphi_j(\mathbf{r}). \end{aligned} \quad (42d)$$

In spherical coordinates the functions $\varphi_i(\mathbf{r})$ can be written

$$\varphi_i(\mathbf{r}) = (u_n(r)/r) Y_{lm}(\theta, \varphi), \quad (43)$$

where n here and in the following denotes all the quantum numbers n , l , and t , of which t is the isotopic spin ($t = -\frac{1}{2}$ for neutron, $t = \frac{1}{2}$ for proton). Thus

$$\mathbf{e}_r \cdot \nabla \varphi_i(\mathbf{r}) = (1/r)(u_n'(r) - (u_n(r)/r)) Y_{lm}(\theta, \varphi), \quad (43a)$$

where u' means the derivative of u , and

$$\nabla^2 \varphi_i(\mathbf{r}) = \frac{1}{r} \left(u_n''(r) - \frac{l(l+1)}{r^2} u_n(r) \right) Y_{lm}(\theta, \varphi). \quad (43b)$$

For filled shells

$$\sum_m Y_{lm}^*(\theta, \varphi) Y_{lm}(\theta, \varphi) = (2l+1)/4\pi. \quad (44)$$

Thus from (42d)

$$\rho(r) = \sum_n ((2l+1)/4\pi) (u_n^2(r)/r^2), \quad (45a)$$

$$\mathbf{e}_r \cdot \nabla \rho(r) = 2 \sum_n \frac{2l+1}{4\pi} \frac{u_n(r)}{r^2} \left(u_n'(r) - \frac{u_n(r)}{r} \right), \quad (45b)$$

$$\rho_2(r) = \sum_n \frac{2l+1}{4\pi} \frac{u_n(r)}{r^2} \left(u_n''(r) - \frac{l(l+1)}{r^2} u_n(r) \right). \quad (45c)$$

These expression together with (42) were used to compute V_a .

By operating with φ_i on (42) we obtain the single-particle potential energy (36) due to the attractive matrix K_a . With (43) we get

$$\begin{aligned} V_{a,n} &= \int V_a^{(0)}(r) u_n^2(r) dr \\ &+ \int V_a^{(1)}(r) u_n(r) \left(u_n'(r) - \frac{u_n(r)}{r} \right) dr \\ &+ \int V_a^{(2)}(r) u_n(r) \left(u_n''(r) - \frac{l(l+1)}{r^2} u_n(r) \right) dr \end{aligned} \quad (46)$$

and

$$P_a = \frac{1}{2} \sum_n (2l+1) V_{a,n}. \quad (47)$$

With the repulsive interaction given by K^I we obtain immediately from (11b)

$$(\mathbf{r}|V^I|\varphi_i) = \frac{3}{4} \gamma \rho^{4/3}(r) / [1 - \delta \rho^{1/3}(r)] \varphi_i(\mathbf{r}), \quad (48)$$

$$V_n^I = \frac{3}{4} \gamma \int \frac{\rho^{4/3}(r)}{1 - \delta \rho^{1/3}(r)} u_n^2(r) dr, \quad (49)$$

and

$$P^I = \frac{1}{2} \sum_n (2l+1) V_n^I \quad (50)$$

or

$$P^I = \frac{3}{8} \gamma \cdot 4\pi \int \frac{\rho^{7/3}(r)}{1 - \delta \rho^{1/3}(r)} r^2 dr \quad (50a)$$

and

$$P = P_a + P^I. \quad (50b)$$

With the repulsive interaction given by K^{II} the evaluation is somewhat more complicated. From (15) we obtain with (37)

$$(\mathbf{r}|V^{II}|\varphi_i) = -\frac{3}{4} c_1 \rho(r) V(r) \varphi_i(\mathbf{r}) - \frac{3}{4} c_1 \sum_j \rho_j(\mathbf{r}) V_j \varphi_i(\mathbf{r}) + \frac{3}{4} c_2 \rho^2(\mathbf{r}) \varphi_i(\mathbf{r}), \quad (51)$$

where V_j was given by (36) and

$$\rho_j(\mathbf{r}) = \varphi_j^*(\mathbf{r})\varphi_j(\mathbf{r}). \quad (51a)$$

After (15) it was pointed out that only diagonal elements of V (15a) should be included. Therefore we can also write

$$\begin{aligned} \langle r | V^{\text{II}} | \varphi_i \rangle = & -\frac{3}{4}c_1 \rho(\mathbf{r}) V_i \varphi_i(\mathbf{r}) - \frac{3}{4}c_1 \sum_j \rho_j(\mathbf{r}) V_j \varphi_i(\mathbf{r}) \\ & + \frac{3}{4}c_2 \rho^2(\mathbf{r}) \varphi_i(\mathbf{r}). \end{aligned} \quad (51b)$$

In an infinite medium when $\rho(r)$ and $V(r)$ are independent of r , Eq. (51) can be used directly. It is probably only for very light nuclei that it is necessary to observe the diagonalization rule, and we still also use (51) instead of the more complicated (51b) in the actual calculations. From (51b) we get the K^{II} contribution to first-order (Hartree-Fock) single-particle energies,

$$V_i^{\text{II}} = -\frac{3}{4}c_1 V_i O_i - \frac{3}{4}c_1 \sum_j V_j O_{i,j} + \frac{3}{4}c_2 O_i', \quad (52)$$

where

$$\begin{aligned} O_i &= \int \rho(r) \rho_i(\mathbf{r}) d\mathbf{r}, \\ O_{i,j} &= \int \rho_i(\mathbf{r}) \rho_j(\mathbf{r}) d\mathbf{r}, \\ O_i' &= \int \rho^2(\mathbf{r}) \rho_i(\mathbf{r}) d\mathbf{r}. \end{aligned} \quad (52a)$$

With φ_i given by (43), adding the attractive part of V we get

$$V_n = \left(V_{a,n} - \frac{3}{4}c_1 \sum_{n'} \frac{2l'+1}{4\pi} V_{n'} O_{n,n'} + \frac{3}{4}c_2 O_n' \right) / (1 + \frac{3}{4}c_1 O_n), \quad (53)$$

where with (43) and (52a)

$$\begin{aligned} O_n &= \int_0^\infty \rho(r) u_n^2(r) dr, \\ O_{n,n'} &= \int_0^\infty u_n^2(r) u_{n'}^2(r) / r^2 dr, \\ O_n' &= \int_0^\infty \rho^2(r) u_n^2(r) dr, \end{aligned} \quad (53a)$$

and $V_{a,n}$ was given by (46). We calculate single-particle potential energies from (53); then the total potential energy is

$$P = \frac{1}{2} \sum_n (2l+1) V_n. \quad (54)$$

With a given set of wave functions $u_n(r)$, the potential energies were thus calculated either from $K_a + K^{\text{I}}$ [P is then given by (50b)] or from $K_a + K^{\text{II}}$ [P given by (54)], and the total energy was got by adding the

kinetic energy

$$T = \sum_n \int_0^\infty (2l+1) u_n(r) \left[u_n''(r) - \frac{l(l+1)}{r^2} u_n(r) \right] dr. \quad (55)$$

Finally the Coulomb energies were added to the single-particle energies and the total energy neglecting the exchange term was obtained.

V. SHELL-MODEL POTENTIAL

As in I, we define the ground state of the nuclear system by the antisymmetrized single-particle wave functions that minimize the total energy with the potential energy given by (35). This defines the wave functions as solutions of a wave equation with a shell-model potential which we shall now derive. The attractive part of the K matrix, K_a , contributes the amount P_a to the potential energy. The variation of the wave functions then gives us the term $\langle r | V_a | \varphi_i \rangle$ of (42). This is of the usual Hartree-Fock type, except that our potential is nonlocal because K_a is nonlocal so that the potential contains ∇ and ∇^2 operators (42).

With the repulsive part of the K matrix given by K^{I} [Eq. (11b)] we obtain a Hartree-Fock-type term in the wave equation which, because of the δ -function range, is simply given by (19), i.e.,

$$\langle r | V^{\text{I}} | \varphi_i \rangle = \frac{3}{4} \gamma \rho^{4/3}(r) / [1 - \delta \rho^{1/3}(r)] \varphi_i(\mathbf{r}). \quad (56)$$

However, K^{I} depends implicitly on the wavefunction φ_i^* through the ρ dependence. Thus we get another term, which we call $V_{K^{\text{I}}}$, since it appears because of a K matrix instead of a simple "static" potential in the potential energy. As shown earlier by Brueckner and Goldman¹¹ it is given by

$$\langle r | V_{K^{\text{I}}} | \varphi_i \rangle = \frac{3}{8} \gamma \rho^2(r) \frac{\partial}{\partial \rho} \frac{\rho^{1/3}(r)}{1 - \delta \rho^{1/3}(r)}, \quad (56a)$$

which gives

$$\langle r | V_{K^{\text{I}}} | \varphi_i \rangle = \frac{1}{8} \gamma \frac{\rho^{4/3}(r)}{[1 - \delta \rho^{1/3}(r)]^2} \varphi_i(\mathbf{r}). \quad (56b)$$

Comparison with (23) gives $V_{K^{\text{I}}} \equiv V_{R^{\text{I}}}$. Thus there is a contribution to the shell-model potential in this case which is just the rearrangement potential. It is a finding after the variation has been performed and not an assumption. The rearrangement energy is by definition a physical removal energy, while the V_K of (56a) is a mere mathematical quantity.

Next, with the repulsive interaction given by K^{II} of Eq. (15), the potential energy is, by (35),

$$\begin{aligned} P^{\text{II}} = & -\frac{9}{16} c_1 \sum_{ijk} \langle \varphi_i \varphi_k | K | \varphi_j \varphi_k \rangle \\ & \times \int \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \varphi_i(\mathbf{r}) \varphi_j(\mathbf{r}) d\mathbf{r} + \frac{3}{8} c_2 \int \rho^3(r) dr. \end{aligned} \quad (57)$$

If we now vary a φ^* we obtain (cf. Ref. 9) a shell-model potential

$$\mathfrak{V}^{\text{II}} = V^{\text{II}} + V_{K^{\text{II}}} \quad (58)$$

and $\langle r | V^{\text{II}} | \varphi_i \rangle$ is given by (51b) while now

$$\langle r | V_{K^{\text{II}}} | \varphi_i \rangle = -\frac{3}{4}c_1 O_i \langle r | V | \varphi_i \rangle - \frac{3}{4}c_1 \sum_j O_j \langle r | S_j | \varphi_i \rangle + \frac{3}{8}c_2 \rho^2(r) \varphi_i(r). \quad (59)$$

Here

$$S_j = \langle \varphi_j | K | \varphi_j \rangle, \quad (59a)$$

i.e., $\sum_j S_j = V$.

The two last terms of (59) are the rearrangement terms for hole and particle interactions. However, the first term, and the first term of (51b) [which by (58) enters into the shell-model potential \mathfrak{V}], appear only because of the prescription to take only diagonal elements of K in K^{II} . If we neglect this prescription we obtain instead of the two terms mentioned only one, i.e.,

$$-\frac{3}{4}c_1 \rho(r) V_i \varphi_i(r) - \frac{3}{4}c_1 O_i \langle r | V | \varphi_i \rangle \rightarrow -\frac{3}{4}c_1 \rho(r) \langle r | V | \varphi_i \rangle, \quad (60)$$

which is just the first term of (51). In an infinite medium this problem does not appear, because then $\rho(r)$ is constant, $O_i = 1$ in Eq. (59), and the first term of (51b) is independent of r and does not affect the wave function but only the meaning of the eigenvalue of the wave function.

Now $V_{K^{\text{II}}} \neq V_{R^{\text{II}}}$ and the eigenvalues of \mathfrak{V} have no apparent physical meaning. This is why in I we stressed that in a variation of a complicated expression for the potential energy like (57) there is no *a priori* reason to believe that the eigenvalues of the wave equation should have any physical meaning.

In a previous work we erroneously included the first term of (51b) in the definition of the rearrangement potential.⁹

In (57) K itself depends implicitly on the wave functions. Thus in (58) we have included the rearrangement

potential only to third order in K , which is just the order to which we have previously calculated it.^{1,18} In an infinite medium we immediately get from (59) the hole-bubble contribution

$$V_{R,h}(k) = -\frac{3}{4}c_1 V(k) \rho, \quad (61)$$

which agrees with (32).

To use the expressions (59) and (51b) in (58) complicates the calculations appreciably because of the dependence of O_i and V_i on the state i whose wave function we are solving for. Iterations have to be performed. Therefore the simpler shell-model potential with the replacement (60) was tried. The goodness of this approximation was tested, as described later.

In our calculations the wave functions $u_n(r)$ will be solutions of an eigenvalue equation

$$(1 + \mathfrak{V}^{(2)}(r)) \left(\frac{d^2 u_n}{dr^2} - \frac{l(l+1)}{r^2} u_n \right) + \mathfrak{V}^{(1)}(r) \left(\frac{du_n}{dr} \frac{u_n}{r} \right) + [\mathfrak{V}^{(0)}(r) + (\frac{1}{2} - l) \mathfrak{V}_c(r)] u_n = E_n u_n, \quad (62)$$

where \mathfrak{V}_c is the Coulomb potential. The potentials \mathfrak{V} are in units of $\hbar^2/2M$. We further introduce the effective mass

$$M^*(r) = 1/[1 + \mathfrak{V}^{(2)}(r)]. \quad (62a)$$

When $K = K_a + K^{\text{I}}$, we obtain from (42), (56), and (56b)

$$\mathfrak{V}^{(2)}(r) = V_a^{(2)}(r), \quad (63a)$$

$$\mathfrak{V}^{(1)}(r) = V_a^{(1)}(r), \quad (63b)$$

$$\mathfrak{V}^{(0)}(r) = V_a^{(0)}(r) + \frac{1}{8} \gamma \rho^{4/3}(r) \{ 6/[1 - \delta \rho^{1/3}(r)] + 1/[1 - \delta \rho^{1/3}(r)]^2 \}. \quad (63c)$$

When $K = K_a + K^{\text{II}}$ and we use the substitution (60), we have with (51)

$$\mathfrak{V}^{(2)}(r) = \frac{V_a^{(2)}(r)}{1 + \frac{3}{4}c_1 \rho(r)} - \frac{3}{4}c_1 \sum_n \frac{2l+1}{4\pi} O_n \left(S_{a,n}^{(2)}(r) - \frac{3}{4}c_1 \rho_n(r) \frac{V_a^{(2)}(r)}{1 + \frac{3}{4}c_1 \rho(r)} \right), \quad (64a)$$

$$\mathfrak{V}^{(1)}(r) = \frac{V_a^{(1)}(r)}{1 + \frac{3}{4}c_1 \rho(r)} - \frac{3}{4}c_1 \sum_n \frac{2l+1}{4\pi} O_n \left(S_{a,n}^{(1)}(r) - \frac{3}{4}c_1 \rho_n(r) \frac{V_a^{(1)}(r)}{1 + \frac{3}{4}c_1 \rho(r)} \right), \quad (64b)$$

$$\mathfrak{V}^{(0)}(r) = \left(V_a^{(0)}(r) - \frac{3}{4}c_1 \sum_n \frac{2l+1}{4\pi} \rho_n(r) V_n + \frac{3}{4}c_2 \rho^2(r) \right) / [1 + \frac{3}{4}c_1 \rho(r)] - \frac{3}{4}c_1 \sum_n \frac{2l+1}{4\pi} O_n \left\{ S_{a,n}^{(0)}(r) - \frac{3}{4}c_1 \rho_n(r) \frac{V_a^{(0)}(r) + V_n + \frac{3}{4}c_2 \rho(r)}{1 + \frac{3}{4}c_1 \rho(r)} \right\}. \quad (64c)$$

Here $S_{a,n}^{(i)}(r)$ is defined by (42a)–(42c) with suppression of the summation over quantum numbers n as in (59a), and

$$\rho_n(r) = u_n^2(r)/r^2. \quad (65)$$

The more exact self-consistent potentials for the interaction $K_a + K^{II}$ are to be used with (58), (51b) and (59) to solve for the functions $u_n(r)$:

$$\mathcal{U}^{(2)}(r) = V_a^{(2)}(r) \left(1 - \frac{3}{4}c_1 O_n\right) - \frac{3}{4}c_1 \sum_{n'} \frac{2l'+1}{4\pi} O_{n'} S_{a,n'}^{(2)}(r), \quad (66a)$$

$$\mathcal{U}^{(1)}(r) = V_a^{(1)}(r) \left(1 - \frac{3}{4}c_1 O_n\right) - \frac{3}{4}c_1 \sum_{n'} \frac{2l'+1}{4\pi} O_{n'} S_{a,n'}^{(1)}(r), \quad (66b)$$

$$\begin{aligned} \mathcal{U}^{(0)}(r) = & \left(V_a^{(0)}(r) - \frac{3}{4}c_1 \sum_{n'} \frac{2l'+1}{4\pi} \rho_{n'}(r) V_{n'} - \frac{3}{4}c_1 \rho(r) V_n + \frac{3}{4}c_2 \rho^2(r) \right) \\ & \cdot \left(1 - \frac{3}{4}c_1 O_n\right) - \frac{3}{4}c_1 \sum_{n'} \frac{2l'+1}{4\pi} O_{n'} (S_{a,n'}^{(0)}(r) - \frac{3}{4}c_1 \rho_{n'}(r) V_{n'} - \frac{3}{4}c_1 \rho V_n + \frac{3}{4}c_2 \rho \rho_{n'}(r)). \end{aligned} \quad (66c)$$

Thus the potentials now depend on the quantum state $n (=nl)$ through V_n and O_n , and one should iterate the solution of the wave equation, as these quantities depend on the solution $u_n(r)$. This will mean added iterations within the major cycle calculating the whole set of $u_n(r)$ and total energy, etc. This iteration was performed, but it was also found that good convergence was obtained by taking O_n and V_n from the previous major iteration.

In the actual computations it was found that the calculation of the potentials $V_a^{(i)}(r)$ according to (42a)–(42c), and especially the partial potentials $S_{a,n}^{(i)}(r)$, required very long computer times. Therefore we tried using an average value of O_n defined by

$$O_{av} = \sum_n (2l+1) O_n / \sum_n (2l+1). \quad (67)$$

This gives a considerable simplification because

$$\sum_n S_{a,n}^{(i)}(r) = V_a^{(i)}(r).$$

For example (64a) then reduces to

$$\mathcal{U}^{(2)}(r) = \frac{V_a^{(2)}(r)}{1 + \frac{3}{4}c_1 \rho(r)} \left(1 - \frac{3}{4}c_1 O_{av}\right) \quad (68)$$

and there are similar simplifications for the rest of the potentials.

In some calculations we also used the potentials (64) and (66) to first order in c_1 . The expansion is straightforward and the expressions are not given here. As pointed out earlier, the potential $V_{K^{II}}$ of (59) is only a lowest order term, the higher orders coming from the fact that K in (57) itself depends on the wave functions. If we work to first order in c_1 we shall replace K in (57) by K_a . There are then no higher order terms and the self-consistent potential is exact within the theory.

VI. SOME COMPUTATIONAL DETAILS

The numerical calculations were made mainly on the CDC 1604 and partly on the CDC 3600 computers of the Computer Center of the University of California at San Diego in La Jolla.

The iterations were started by guessing or taking from some previous calculation the shell-model potentials $\mathcal{U}^{(i)}(r)$ as well as the Coulomb potential. Then the eigenfunctions were obtained by solving the wave equation (62) with a fourth order Runge-Kutta scheme. The integrations were started from outside at some radius large enough so that the potentials were negligibly small. At this point the logarithmic derivative is $u_n'(r)/u_n(r) = (E_n)^{1/2}$. The eigenvalue E_n was obtained by the condition $u_n(0) = 0$. A method was developed that counted the nodes and maxima and minima of the wave function, so that with n specified the eigenvalue was automatically corrected to give the proper eigen-solution $u_n(r)$. In the integrations the mesh 0.2 F was found quite sufficient.

With the wave functions $u_n(r)$ given, the energies were calculated by the proper expressions previously derived. When doing the integrations (42a)–(42c) the mesh in the angular integration $d(\cos\theta)$ was 1/13 and in the radial integration it was 0.2 F. All integrations were made by Simpson's rule.

When using the K^{II} matrix the potential energies V_n were calculated from (53) by iteration. In the first iteration we put $V_{n'} = V_{a,n} + c_2 O_{n'}$, which is of zero order in c_1 . Then the iterations were repeated until the potential energy per nucleon obtained from (54) changed less than 0.02 MeV between two successive iterations. This took about four iterations.

Finally, new shell-model potentials were computed as described and the major iterations were repeated until the root-mean-square change in density was less than 0.001 F⁻³ between two successive iterations. With a sensible first guess the number of iterations required was three to five.

With the functions $v_0(r)$ and $v_2(r)$ in (1) given by δ -functions, whence the integrations in (42a–c) are made analytically, the time for each iteration on the CDC 1604 was about 15 sec for O¹⁶ and 30 sec for Ca⁴⁰. With $v_0(r)$ and $v_2(r)$ defined by (10a) the time increased considerably especially because the integrations (42a–c) had to be performed repeatedly to obtain the $S_{a,n}^{(i)}$ in

(64) and (66). In O^{16} and with K^I , i.e., potentials (63), each iteration was 1 min 30 sec and with K^{II} , i.e., potentials (64), each iteration was 7 min 30 sec. In Ca^{40} they were, respectively, 2 and 14 min.

With the averaging (67) the times were reduced to 1 min 40 sec and 2 min 30 sec for O^{16} and Ca^{40} , respectively.

On the CDC 3600 these times were divided by about five.

VII. TEST OF APPROXIMATIONS

We wish to show results for the test of approximations that we used.

First we tested the approximation of using the potentials (64) instead of the more self-consistent (66). We then used these potentials expanded to first order in c_1 . Further, we used δ -function interactions. Then the calculations become sufficiently accurate that we expect (66) to be exact self-consistent, i.e., give numerically the exact minimum in total energy. On the other hand, we expect (64) to give slightly less binding. The test was made on O^{16} , since we expect this approximation to be worst for a small nucleus. The result is shown in Table I, run numbers 1 and 2. We find that

TABLE I. Test of approximations. KE=kinetic energy. PE=potential energy. E =total energy. A =number of nucleons. R =root-mean-square radius. Units: Fermi and MeV. Nucleus: O^{16} .

Run No.	E/A	R	KE/A	PE/A	Potential
1	-15.01	2.12	23.76	-38.77	(64) to order c_1
2	-15.09	2.17	22.64	-37.73	(66) to order c_1
3	-7.49	2.43	17.92	-25.41	(64)+(67)
4	-7.46	2.44	17.64	-25.10	(64)

the error in binding is less than 0.1 MeV and in the radius (by which we shall always mean the root-mean-square radius) 0.05 F. The exact potentials (66) are effectively more repulsive.

As pointed out earlier, the energy eigenvalues of potentials (66) have no apparent physical meaning. They are now not identical to separation energies. However, we can also calculate these separation energies by adding to the first-order K -matrix energies the rearrangement energies. This was also done and is presented in Table II (run 2). With potentials (64), the eigenvalues are not exactly the separation energies either, but the difference is very small and we do not

TABLE II. Comparison of eigenvalues and separation energies in O^{16} .

Run No.	State	Neutron		Proton	
		Separation energy	Eigenvalue	Separation energy	Eigenvalue
2	1s	-70.54	-51.94	-65.08	-46.71
	1p	-34.49	-24.85	-29.56	-20.21
1	1s		-69.11		-63.51
	1p		-31.93		-26.88

distinguish between them. We do find the eigenvalues of run 2 appreciably higher than the separation energies and than the eigenvalues of run 1. Actually we find from (64) that the difference between them is $O_n V_n$.

The results of Table I lead us to accept the approximate potentials (64) as good, at least when working to first order in c_1 , i.e., to first order in the short-range correlation. Also, however, when we calculate the energy to all orders in c_1 the $V_{K^{II}}$ of (59) is only a first order term in c_1 , as pointed out earlier. We found that this resulted in a too large rearrangement energy at the Fermi surface and presumably in all states (31), (32). Therefore the use of the approximation (64), which from Table I is found to be slightly too attractive, and the first order $V_{K^{II}}$ gives cancellation of errors to some extent.

To save further computation time we also wished to use the averaging (67) of O_n . In an infinite medium $O_n = \rho = \text{constant}$ and (67) is exact. Therefore the approximation should again be worse for O^{16} (compared to Ca^{40}). We now (and in the following) use the interactions (10a), i.e., a finite range. In Table I, runs 3 and 4, the result is shown. Again the error is much smaller than we in fact had reason to expect. Actually the binding is *increased* by the approximation and its value is thus within the limits of the errors of the preceding approximations.

Most of the calculations now to be presented are calculated with the potential (64) modified by (67). Thus we expect our approximations to give us the binding to within ~ 0.1 MeV and the radius to within ~ 0.1 F. Further indirect tests of these approximations are obtained later.

The K^I matrix is simple enough that no approximations were required in potentials (63).

VIII. COMPARISON OF K^I AND K^{II} REPULSIONS

A main purpose of this investigation was to compare the results for the local density approximation (K^I matrix) with the results for the more detailed K^{II} matrix. The results of this comparison are presented in Tables III and IV. The functions $v_0(r)$ and $v_2(r)$ were those of (10a). The parameters of the interaction were "normalized" as described in Sec. III so that the infinite system saturates of $\rho = 0.1948 \text{ F}^{-3}$ with a binding energy 15.5 MeV/particle.

With the core parameters γ and δ given by (11d), we find for O^{16} (run 5) and Ca^{40} (run 6) bindings of 3.43 and 4.78 MeV/particle, respectively. These are to be compared with the Brueckner-Lockett-Rotenberg (BLR) values 2.02 and 3.89 MeV/particle. Although the repulsive core term of their calculation is, apart from the spin averaging, identical to ours, we have used a very simplified attractive interaction and worked in the effective-mass approximation. Thus the agreement between the BLR results and ours is satisfactory. We think the agreement justifies further comparisons.

TABLE III. Calculations with K^I repulsion (local-density approximation). Units are MeV and F.

Run No.	Nucleus	E/A	R	Shell-model potential	α	β	γ	δ
5	O ¹⁶	-3.43	2.68	Self-consistent Eq. (63)	1.061	0.351	202.6	0.763
6	Ca ⁴⁰	-4.78	3.28					
21	O ¹⁶	-3.36	2.52	Eq. (63), but without rearrangement term	1.061	0.351	202.6	0.763
22	Ca ⁴⁰	-4.69	3.10					
27	O ¹⁶	-3.41	2.63	Gauss: $V_0 = -77.8$ $\nu = 0.206$				
7	O ¹⁶	-3.25	2.68	Self-consistent: Eq. (63)	1.027	0.309	170.4	0.916
8	Ca ⁴⁰	-4.62	3.28					
9	O ¹⁶	-3.53	2.68	Self-consistent: Eq. (63)	1.084	0.376	229.1	0.636
10	Ca ⁴⁰	-4.87	3.28					

The BLR radii were 2.56 and 3.01 F, respectively, for O¹⁶ and Ca⁴⁰.

In order to see how sensitive the binding is to the exact values of the parameters γ and δ , we also changed δ by 20% and recalculated γ to give the same repulsive contribution to the potential energy in the infinite system, 15.35 MeV/particle (and changed α and β to give the same saturation). The result is runs 7-10. The binding is changed by less than 5% and the radii are unchanged. Thus the exact values of γ and δ are not critical, as long as the total repulsion is unchanged.

We then used the repulsion K^{II} . First we assumed $c_2=0.0$ and calculated from (28) the value of c_1 that gave the above repulsive contribution to the potential energy (15.35 MeV/particle). We find $c_1=1.295$, which is somewhat higher than the value of this parameter (14) discussed in I. We then found the binding energies presented in runs 11-12. Thus the binding is increased, compared to the local density calculations of runs 5 and 6, by about 2.5 MeV for O¹⁶ and 2.2 MeV for Ca⁴⁰, while the radii are decreased slightly. The increase in binding is in agreement with our previous qualitative discussions.^{1,9}

The lower limit of c_1 previously discussed is $c_1=0.5$. Assuming this value of c_1 we compute from (28) the value $c_2=521.5$ MeV F⁶ to give the above repulsive

energy 15.35 MeV. This value of c_2 is rather large. Our estimate gives (with an effective mass for the excited states of 0.77 M) a value $c_2=311$ MeV F⁶. As discussed in I, the term proportional to c_2 (particle-bubble interaction) depends on the local density like the K^I repulsion. Further, owing to the density-squared term in (28) we expect the binding to decrease appreciably. The calculation is shown in runs 13 and 14. The binding does decrease by 1.6 and 1.4 MeV for O¹⁶ and Ca⁴⁰, respectively, compared to runs 11 and 12. Although the value of c_2 is very large, the binding is about 0.8 MeV larger than for the local-density K^I repulsion. For comparison, we also calculated with $c_1=0.5$ but $c_2=0$ (runs 15 and 16) which shows that the main decrease in binding in runs 13 and 14 is due to the repulsive term proportional to c_2 .

It is of some interest to see explicitly the effect the medium-dependent core repulsion has on the binding. Therefore we put $c_1=c_2=0$ (or $\gamma=0$) and obtained runs 17 and 18. If we now look also at runs 5 and 11 for O¹⁶ and runs 6 and 12 for Ca⁴⁰, we see that with $c_2=0$ the K^{II} repulsion increases the binding but the K^I repulsion decreases it. This may be explained by noting that the repulsion in K_a (the ∇^2 term) is more "local" than the K^{II} repulsion with $c_2=0$ but less local than the K^I repulsion. We may also state the result of

TABLE IV. Calculations with K^{II} repulsion ("exact" core treatment). Units are MeV and F.H.O.=harmonic oscillator.

Run No.	Nucleus	E/A	R	Shell-model potential	α	β	c_1	c_2
11	O ¹⁶	-5.90	2.48	Self-consistent: Eqs. (64), (67)	1.120	0.419	1.295	0.0
12	Ca ⁴⁰	-7.01	3.12					
12a	Ca ⁴⁰	-7.07	3.15	As above but modified Eq. (69)	1.120	0.419	1.295	0.0
19	O ¹⁶	-5.79	2.55					
20	Ca ⁴⁰	-6.89	3.20	H.O.: $\nu=0.39$	1.120	0.419	1.295	0.0
23	O ¹⁶	-5.80	2.40					
24	Ca ⁴⁰	-7.11	3.09	H.O.: $\nu=0.305$	1.120	0.419	1.295	0.0
25	O ¹⁶	-6.00	2.43					
26	Ca ⁴⁰	-7.15	3.13	Gauss: $V_0 = -79.8$ $\nu = 0.255$ $\nu = 0.212$				
13	O ¹⁶	-4.27	2.57	Self-consistent: Eqs. (64), (67)	1.003	0.283	0.667	521.5
14	Ca ⁴⁰	-5.62	3.19					
15	O ¹⁶	-5.75	2.46	Self-consistent: Eqs. (64), (67)	1.080	0.492	0.667	0.0
16	Ca ⁴⁰	-6.79	3.12					
17	O ¹⁶	-5.54	2.45	Self-consistent: Eqs. (64), (67)	1.040	0.569	0.0	0.0
18	Ca ⁴⁰	-6.52	3.12					

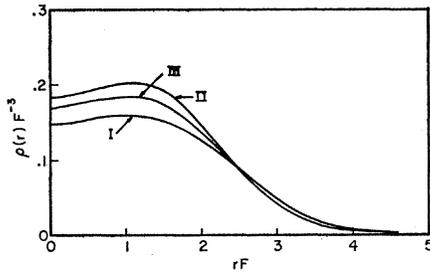


FIG. 1. Density distributions in O^{16} . I: K^I repulsion (run No. 5), II: K^{II} repulsion (run No. 11), III: K^{II} repulsion, but an approximate second-order K -matrix term included in the shell-model potential (run No. 19).

this calculation as that the effect of the hole-bubble third order K -matrix graph is to decrease the surface energy.

TABLE V. Separation energies for O^{16} in MeV. n and p refer to neutron and proton states, respectively.

Run No.	5	11	19	25
Repulsion	K^I	K^{II}	K^{II}	K^{II}
Shell-model potential	Self-consistent Eq. (63)	Self-consistent Eqs. (64), (67)	As before but modified Eq. (69)	Gauss: $V_0 = -79.8$ $\nu = 0.255$
State				
$1s, n$	-36.2	-45.0	-35.0	-46.0
$1s, p$	-31.6	-40.0	-30.1	-40.9
$1p, n$	-15.6	-19.7	-17.4	-19.9
$1p, p$	-11.7	-15.5	-13.2	-15.5

In Tables V and VI are shown separation energies for the K^I and K^{II} repulsions. The K^I separation energies are somewhat larger than those tabulated by BLR. However, these tables are for a decreased repulsion. In agreement with the larger binding for the K^{II} repulsion, the separation energies are also larger for this repulsion. However, the agreement with experiments for the top nucleons and especially for the proton-neutron difference seems surprisingly good.

In Figs. 1 and 2 are shown density distributions for O^{16} and Ca^{40} with the K^I and K^{II} repulsions. The K^{II} repulsion, being effectively less repulsive, gives larger central densities, but the distributions have the same general shape.

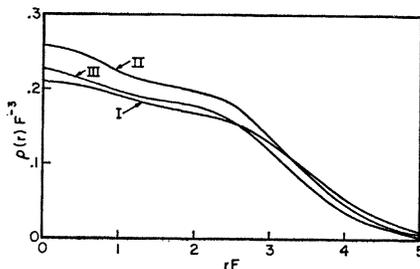


FIG. 2. Density distributions in Ca^{40} . I: K^I -repulsion (run No. 6), II: K^{II} repulsion (run No. 12), III: K^{II} repulsion, but an approximate second-order K -matrix term included in the shell-model potential (run No. 20).

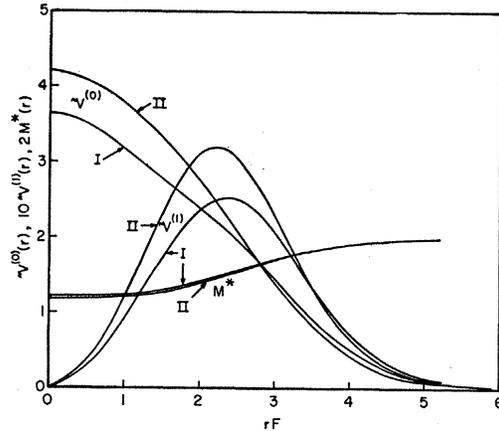


FIG. 3. Self-consistent shell-model potentials for O^{16} . I: K^I repulsion (run No. 5), potentials defined by Eq. (63). II: K^{II} repulsion (run No. 11), potentials defined by Eq. (64).

Also the potential functions shown in Figs. 3 and 4 show the same general behavior, but K^{II} gives some-

TABLE VI. Separation energies for Ca^{40} in MeV. n and p refer to neutron and proton states, respectively.

Run No.	6	12	20	26
Repulsion	K^I	K^{II}	K^{II}	K^{II}
Shell-model potential	Self-consistent Eq. (63)	Self-consistent Eqs. (64), (67)	As before but modified Eq. (69)	Gauss: $V_0 = -79.8$ $\nu = 0.212$
State				
$1s, n$	-55.6	-63.2	-48.0	-65.7
$1s, p$	-48.1	-53.3	-38.4	-55.3
$1p, n$	-35.8	-40.7	-32.6	-41.2
$1p, p$	-27.3	-31.6	-23.8	-31.8
$1d, n$	-17.6	-19.9	-18.0	-19.6
$1d, p$	-10.0	-11.9	-10.1	-11.3
$2s, n$	-15.7	-18.5	-16.9	-19.0
$2s, p$	-8.3	-10.6	-9.0	-10.6

what larger values corresponding to the larger densities, as shown by Figs. 1 and 2.

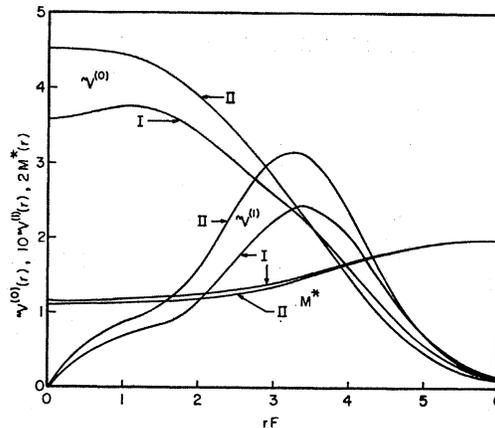


FIG. 4. Self-consistent shell-model potentials for Ca^{40} . I: K^I repulsion (run No. 6), potentials defined by Eq. (63). II: K^{II} repulsion (run No. 12), potentials defined by Eq. (64).

IX. THE SELF-CONSISTENT POTENTIAL

In I we calculated rearrangement energies and found that the second order rearrangement term was strongly nonlocal, especially owing to the long-range part of the central interaction. We have not included in this investigation any medium dependence of the long-range interaction. It is, however, of interest to see how the addition of such a nonlocal potential to the shell-model potential affects the density distribution. We therefore modified the functions $\mathcal{U}^{(0)}(r)$ and $\mathcal{U}^{(2)}(r)$ accordingly:

$$\mathcal{U}^{(0)}(r) \rightarrow \mathcal{U}^{(0)}(r) + 5.064\rho(r), \quad (69a)$$

$$\mathcal{U}^{(2)}(r) \rightarrow \mathcal{U}^{(2)}(r) - 0.840\rho^{1/3}(r), \quad (69b)$$

corresponding roughly to our calculations of the second-order rearrangement potential in I. These additions do not change the potential of the Fermi surface in an infinite medium. The result is presented in runs 19 and 20. The effect of this addition to the potentials is seen to be very small. The binding decreases by only 0.1 MeV and the radius increases by around 0.1 F. In Figs. 1 and 2 it is shown how the inclusion of the second-order rearrangement potential reduces the central densities by 0.02 F^{-3} in O^{16} and 0.03 F^{-3} in Ca^{40} .

Although the change in energy and size is small, the separation energies do change by several MeV, as seen in Tables V and VI.

As a change in the shell-model potential by an amount of the order of the potential V_K or the rearrangement potential affects the calculations so little, we also think it is of interest to see the effect of completely neglecting V_K in the shell-model potential. This is done in runs 21 and 22. In these calculations were included only the first order K matrix or the Hartree-Fock potential. The binding is reduced by less than 0.1 MeV and the radius by less than 0.2 F. This result is thus in disagreement with BLR, who find that the inclusion of the rearrangement potential is very important.

It is quite simple with our interaction to check the importance of the rearrangement potential for saturation of an infinite system, by applying the expression (33) at saturation. The neglect of V_K in a finite nucleus corresponds to neglecting the rearrangement potential in the single-particle potential $\mathcal{U}(k_F)$. With the K^I interaction we then get

$$k_F^2 + V_a(k_F) + V^I = 0.6k_F^2 + P_a + P^I, \quad (70)$$

where V_a , V^I , P_a , and P^I are given by Eqs. (16a), (19), (18a), and (20), respectively. With the parameters given as in runs 5 and 6, the saturation density is 0.1948 F^{-3} with a binding 15.5 MeV [as obtained by adding the rearrangement potential (23) on the left-hand side of (70)].

Solution of (65) for k_F gives a density 0.256 F^{-3} and the binding energy is then 13.3 MeV/particle. The central density in run 22 is 0.26 F^{-3} . Thus the neglect

of the rearrangement potential increases the density by 0.05 F^{-3} , as seen from Fig. 2. The decrease in binding energy is much smaller for the finite nucleus than for the infinite. Probably this is because of the regions of low density in the finite nucleus where the repulsive force is less effective.

Our interaction gives a considerably smaller compressibility than the Brueckner-Gammel potential. The energy of our system increases especially rapidly with compression. This is quite certainly because of the effective-mass approximation. Our system is too stiff, especially as regards density increase. This now explains why we found the inclusion of the V_K potential unimportant in our calculations. This result might not be true for a realistic K matrix, as was also found by BLR.

X. LOCAL SHELL-MODEL POTENTIALS

The derivation of the self-consistent shell-model potential that we have used involves in principle, as previously pointed out, a variation of an infinite number of parameters (i.e., the wave functions at all points in space) to minimize the total energy. We do, however, know that a nucleus consists mainly of a central and a surface region, and we expect that it would really be sufficient to minimize the energy only with respect to a few parameters that describe these properties. The most important ones would, e.g., be a radius and a surface thickness.

In previous shell-model calculations one has often with apparent success used harmonic-oscillator wave functions for light nuclei. Such wave functions have also been used in previous calculations^{9,16} using K -matrix theory on the binding of O^{16} .

We decided it to be of interest to try some simple local potentials. We minimized the energy of O^{16} and Ca^{40} with respect to the one parameter of the harmonic oscillator (H.O.) potential and the two parameters of the Gaussian. We think the result was somewhat surprising. With a H.O. potential $V = \nu^2 r^2$ we obtained the results of runs 23 and 24, and with a Gaussian potential $V = V_0 e^{-\nu^2 r^2}$ those of runs 25 and 26. These are to be compared with the runs 11 and 12a using self-consistent potentials. Run 12a is almost the same as 12. For technical reasons we started the integration of the wave equation further out with the local potentials of Ca^{40} , than had been done in previous runs. The same integration was done in 12a as with the local potentials.

We see that the bindings are within 0.1 MeV of the bindings obtained using the self-consistent potential. Moreover, to our surprise, the bindings with the local potentials are even larger for Ca^{40} and for O^{16} with the Gaussian potential. This may seem strange, since the self-consistent potential is *defined* to minimize the energy, yet with the local potentials we can obtain wave

¹⁶ R. J. Eden and V. J. Emery, Proc. Roy. Soc. (London) A248, 266 (1958); R. J. Eden, V. J. Emery, and S. Sampanthar, *ibid.* A253, 177, 186 (1959).

functions that give even lower energy. However, the potential V_K of Eq. (59), is, as previously discussed, only a first-order correction. Further, we did have to approximate somewhat in the exact self-consistent potential, in order to make the computations reasonably short. And in fact we found that the error that these approximations give would be of the order of 0.1 MeV (Sec. VII), which is just the increased binding we are able to obtain.

In order to check to some extent that the larger binding was not due to some error in the calculations, we also used a local shell-model potential with the K^I repulsion of run 5. With this K matrix, no approximation on the self-consistent potential is necessary, and the computation is exact, i.e., should give the absolute maximum binding. With a Gaussian we obtained run 27. Thus the binding is now *smaller*, as it ought to be unless our calculation were in error. We note, however, that the difference is only 0.02 MeV, which would thus be the error in binding obtained by the use of a local instead of a nonlocal potential.

Our results thus show that in order to calculate the binding of a light nucleus like O^{16} or Ca^{40} it is quite adequate to use a H.O. (local) shell-model potential to compute the wave functions. There is no reason to believe that our results should depend on the special kind of K matrix we have been using.

We regard this finding as important for practical reasons because:

(A) In an exact calculation of the K matrix, this matrix depends in a quite involved way on the single-particle wave functions and the calculation of any self-consistent shell-model potential will then be quite intricate. This is especially so because of the Pauli principle, which gives complicated second-order rearrangement terms.

(B) Even if we can obtain a shell-model potential, it will be rather involved for practical calculations. In fact, in the above calculations we had to approximate our potentials, which resulted in errors in the binding which for Ca^{40} were actually larger than those involved in using the local H.O. potential.

(C) In the exact treatment of the K matrix we do not expect that the effective-mass approximation will be numerically acceptable. Thus if we derive a shell-model potential, it will have a more general nonlocal structure, and we shall have to solve the general integro-differential equation as was done by BLR. This is a quite tedious computation and BLR actually used approximate procedures also at this point.

(D) The H.O. wave functions are simple and provide an easy separation into center-of-mass and relative motion.

In fact, as pointed out earlier, we used the H.O. set of wave functions in an earlier calculation⁹ on O^{16} and we are, by virtue of the investigation presented in this paper, able to state the goodness of that procedure as

far as the calculation of energy by H.O. functions is concerned. We then obtained a binding of 3.4 MeV/nucleon. This is larger than the binding obtained by BLR but less than the binding obtained in this investigation, although we did include a repulsion of the type K^{II} . However, the nucleon potential we used gives only 11.5-MeV binding per particle in the infinite system. At least 10% more potential energy is necessary to give 15.5 MeV/particle, and that would give around 5.5 MeV/particle in O^{16} . To compare the H.O. results with our present calculations we should also, as shown in Sec. XI, subtract about 0.76 MeV from this value to get around 4.7 MeV/nucleon. This is about 1 MeV smaller than the result of run 15, which has the repulsion most similar to the one in Ref. 9. The difference must thus be due to the use of the effective-mass approximation, and this conclusion is roughly justified by the difference of 1.4 MeV/nucleon between our run 5 and the BLR binding for O^{16} .

Of course the use of a local shell-model potential instead of a truly self-consistent potential to calculate the energy is feasible only because our criterion for a good approximation to the energy is that we get a good approximation both to the energy *and* to the density distribution when the energy is minimized. As we pointed out previously here and in I, this criterion is of a numerical nature and may involve a calculation of higher order graphs specifically important in a light nucleus. Even though the correlations in the nucleus thus may be more complicated⁶ than the original Brueckner K -matrix theory assumes, we still believe that the H.O.-model wave functions are adequate for light nuclei and may actually make the calculation of these correlations numerically possible.

In line with our earlier discussions, it is not necessarily true that a good calculation of the binding well describes (within the theory) other properties such as density distributions. A comparison of densities from the self-consistent potential with those from the H.O. and Gaussian potentials is given in Figs. 5 and 6. We see that there is an appreciable difference in central densities, especially for Ca^{40} . The local potentials give larger central densities, with the exception of the H.O. for O^{16} . This may be a general property of local as com-

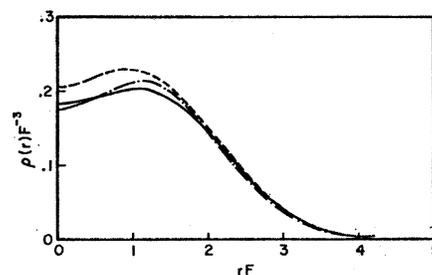


FIG. 5. Density distribution in O^{16} with K^{II} repulsion. Full line: Self-consistent potential (run No. 11), same as Fig. 1, curve II. Broken line: Gaussian local potential (run No. 25). Dotted line: harmonic oscillator local potential (run No. 23).

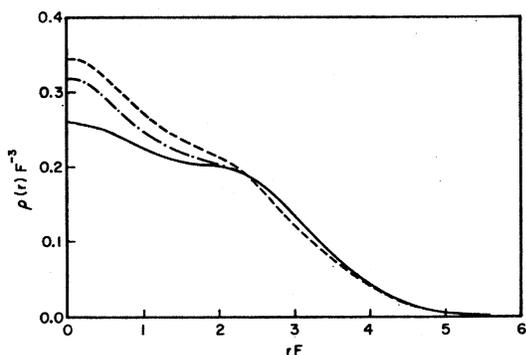


FIG. 6. Density distribution in Ca^{40} with K^{II} repulsion. Full line: Self-consistent potential (run No. 12), same as Fig. 2, curve II. Broken line: Gaussian local potential (run No. 26). Dotted line: Harmonic oscillator local potential (run No. 24).

pared to a nonlocal potential, although we do not wish to stress this point. However, in Figs. 7 and 8, where the wave functions for the self-consistent potential are plotted along with those for the Gaussian, we do find that the former are slightly less curved and pushed out, which may be because the nonlocality damps the curvature, especially at the center of the nucleus where the effective mass is smallest.

Although the Gaussian potentials, because of the approximations in the self-consistent ones, give more binding, the density distributions given by the former are probably less exact than those given by the latter potentials, although we cannot state this with certainty.

The energy eigenvalues of the wave functions for our local H.O. or Gaussian potentials have of course no meaning whatsoever in our theory. However, given the wave functions we can calculate the separation energies as the sum of a first and a third order K -matrix graph. The result is given in Tables V and VI for the Gaussian potentials. The agreement with the proper K^{II} repulsions (runs 11 and 12a) is remarkably good.

If a good approximation to the self-consistent potentials can be made, one can also use, e.g., the H.O. wave functions obtained by minimizing the energy to calculate these self-consistent potentials. By solving for the eigenfunctions we can then obtain a density distribution that is more exact than that given by the H.O. wave functions. This procedure is of practical use if: (i) it is of advantage to calculate an exact K matrix

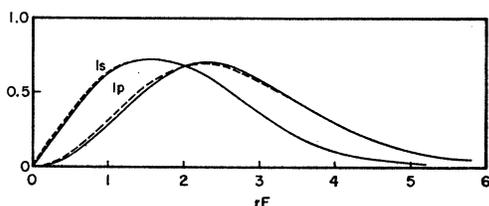


FIG. 7. Neutron wave functions for O^{16} . Full line is for self-consistent potential (run No. 11), broken line for Gaussian local potential (run No. 25).

with H.O. wave functions rather than from some general ones; (ii) the convergence is fast enough so that one iteration is sufficient with the self-consistent potential after the energy has been minimized with a H.O. potential. Point (ii) has been investigated. Although the Gaussian and self-consistent potentials give such different density distributions, we find one iteration suffices to bring the central density down from 0.345 to 0.263 F^{-3} , i.e., to the self-consistent value. Point (i) is presently under investigation.

XI. COMPARISON WITH EXPERIMENTS

The experimental energies¹⁷ and root-mean-square radii¹⁸ are

$$\text{for } \text{O}^{16}: \quad E/A = -7.98 \text{ MeV} \quad R = 2.57 \text{ F};$$

$$\text{for } \text{Ca}^{40}: \quad E/A = -8.55 \text{ MeV} \quad R = 3.49 \text{ F}.$$

Actually we cannot directly compare the experimental bindings with those we calculated. In the calcu-

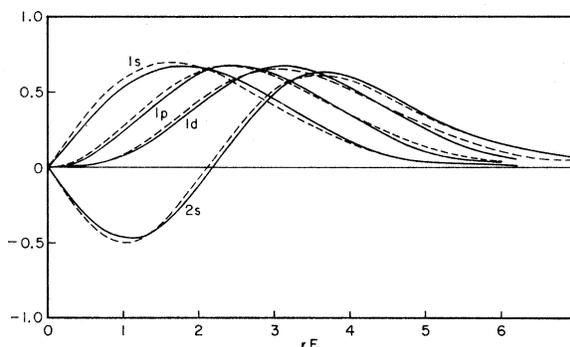


FIG. 8. Neutron wave functions for Ca^{40} . Full line is for self-consistent potential (run No. 12a), broken line for Gaussian local potential (run No. 26).

lations the nucleon motions are calculated in a fixed potential well, which means implicitly that the center of mass is in a state of motion. Thus we have to subtract the energy associated with this center-of-mass motion. This can be done explicitly for H.O. states.¹⁹ In the ground state the center of mass is in a 1s state the kinetic energy of which is $\hbar^2\nu/2M$. Thus the correction to our calculation is with the ν values we found for O^{16} and Ca^{40} : -0.76 and -0.23 MeV/nucleon, respectively. This correction is thus not negligible for O^{16} . We have in all calculations "normalized" our K matrix to make the infinite medium saturate at $k_F = 1.42 \text{ F}^{-1}$ with an energy -15.5 MeV/nucleon, which is close to the experimental values and the result obtained by Brueckner and Gammel.²

The K matrix used in this paper is too simplified to warrant any direct comparison with experiments. How-

¹⁷ A. H. Wapstra, *Physica* **21**, 367, 385 (1955).

¹⁸ D. G. Ravenhall, *Rev. Mod. Phys.* **30**, 430 (1958).

¹⁹ J. P. Elliott and T. H. R. Skyrme, *Proc. Roy. Soc. (London)* **A232**, 561 (1955).

ever, we find from Tables III and IV that our treatment of the core term increases the binding relative to the BLR result by about 2–2.5 MeV. BLR obtained 2.02 and 3.89 MeV/nucleon for O^{16} and Ca^{40} , respectively. Including our center-of-mass correction we still have to account for about 2–3 MeV/nucleon binding. We expect to be able to calculate the binding theoretically to within 1 MeV. So there is still a discrepancy between theory and experiment.

In I, we claimed to have shown that not only the core but also the long-range correlation depends on the nuclear structure. Especially we claimed that this is so for the tensor force. In fact the long-range correlation increases with decreasing density, and so relatively increases the binding for small densities and finite nuclei.

In Ref. 9 we calculated with H.O. wave functions the binding of O^{16} . We then also included a second-order Born term, i.e., a long-range correlation term. This contributed 1.16 MeV/nucleon to the binding. At normal density of an infinite system the same term contributes³ 0.8 MeV. The energy due to a medium-independent force in the same calculations is about half in O^{16} of what it is in an infinite medium. Thus these calculations already show that the long-range correlations would increase the binding in O^{16} by roughly $1.16 - \frac{1}{2} \times 0.8 = 0.76$ MeV/nucleon. The quoted calculations did not properly treat the off-energy-shell effect, which might appreciably decrease this value. However, the tensor force correlations are much stronger, and we think this may very well increase the binding for a finite nucleus by the necessary 2 MeV or so.

Our H.O. parameters ν agree well with the relation of Moszkowski,²⁰ $(\hbar^2/M)\nu = 41A^{-1/3}$ MeV, which gives $\nu = 0.39$ and $\nu = 0.29$ for O^{16} and Ca^{40} , respectively, (runs 23 and 24 give $\nu = 0.39$ and $\nu = 0.31$).

XII. CONCLUDING REMARKS

We think this investigation throws some light on the K -matrix theory of finite nuclei.

In Sec. VIII we showed that a more detailed treatment of the core repulsion than that of BLR increases the binding by several MeV.

It is now, in principle, necessary to distinguish be-

²⁰ S. A. Moszkowski, *Handbuch der Physik*, edited by S. Flügge (Julius Springer-Verlag, Berlin, 1957), Vol. 39, p. 441.

tween three different single-particle energies. The K -matrix definition contains virtual energies so defined as to implicitly sum important K -matrix graphs. The shell-model potential defines further eigenvalues of the shell-model wave functions. Neither of these potential energies has any physical meaning. The separation energy, on the contrary, is defined as the energy needed to physically remove a particle. The main parts of all these single-particle energies are of first order in the K matrix. In fact our calculations in Sec. IX show that the binding energy and density distributions are relatively insensitive to the self-consistent potential. The main part of the self-consistent potential is the first order K -matrix part or Hartree-Fock potential. We found that this part of the potential already gave the binding to within about 0.2 MeV/nucleon and the radius to within about 0.2 F. Thus the energy of a finite nucleus is less sensitive to the neglect of higher order terms in the self-consistent potential than it is in an infinite medium, because neglecting the rearrangement term decreases the binding by about 2 MeV in the latter case.

In Sec. X we found that a local H.O. shell-model potential is sufficient for calculating binding energies, probably to within about 0.2 MeV. These calculations do indicate, however, that the local potential is not properly adequate for calculating density distributions.

As pointed out in Sec. XI, there is still a discrepancy between theoretical and experimental binding energies for the light nuclei, as calculated by a first order K matrix, "normalized" to saturate the infinite medium as deduced experimentally. The agreement will probably be better if the long-range correlations are treated properly, and it does now seem reasonable to hope that the Brueckner theory of nuclear matter with Bethe's improved treatment of 3-body interactions will adequately describe the binding of finite nuclei also.

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