

Modified Hartree-Fock Method for the Finite Nucleus*

K. A. BRUECKNER† AND D. T. GOLDMAN

Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania

(Received June 1, 1959)

A procedure is given for including the rearrangement energy term in the Brueckner-Gammel method for evaluating the structure of finite nuclei. A variational technique is used to derive the single-particle energy from the total binding energy of the nucleus.

It is seen that although a rearrangement energy term does not appear explicitly in the total nuclear binding energy, it is derivable from the binding energy and influences the eigenfunctions of the total nuclear system, and thus its energy eigenvalues. The rearrangement energy has a noticeable effect on the single-particle wave equation and must be included in finite nucleus calculations. To a good approximation, it is shown that it is possible to evaluate the rearrangement potential and to express it as a simple function of the mean nuclear density, i.e.,

$$V_R = (240 \text{ Mev})\rho^2 \times (10^{-13} \text{ cm})^6.$$

A METHOD has been described¹ for determining the structure of finite nuclei by a modified Hartree-Fock procedure. This method is based on the approximation that the local correlation structure of a finite nucleus is identical to that of nuclear matter at the same local density. In this approximation, which is discussed extensively in I, the effective particle-particle interaction in the finite system is the nonlocal K -matrix

$$(\mathbf{r}_{12} | K(\rho) | \mathbf{r}_{12}'), \quad (1)$$

which is determined from the self-consistent K -matrix evaluated in the study of nuclear matter by Brueckner and Gammel.² The density ρ appearing in the K -matrix is an average density over the correlation range and may approximately be taken to be that at the center of gravity of the two interacting particles,

$$\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2.$$

The K -matrix of Eq. (1) can be considered to be the operator whose matrix element taken with respect to the eigenstates of the finite system determines the energy. Our problem is to determine the form of the eigenstates, the energy eigenvalues, and other nuclear parameters.

We start by defining an orthonormal set of single-particle states $\psi_i(\mathbf{r}_i)$ of a form to be determined. The model wave function for the system then is

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = A\psi_1\psi_2(\mathbf{r}_1) \cdots \psi_N(\mathbf{r}_N), \quad (2)$$

where A is the antisymmetrizing operator and N is the total number of particles in the system. The effective Hamiltonian for the system is

$$H = \sum_{j=1}^N \frac{p_j^2}{2m} + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N (\mathbf{r}_{ij} | K(\rho) | \mathbf{r}_{ij}'), \quad (3)$$

* Supported in part by a grant from the National Science Foundation.

† Present address: University of California, La Jolla, California.

¹ Brueckner, Gammel, and Weitzner, Phys. Rev. **110**, 431 (1958). We shall refer to this paper in the following as I.

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

where

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j.$$

The expectation value of H taken with respect to Ψ is

$$\begin{aligned} W = \langle H \rangle &= \sum_{i=1}^N \int \psi_i^*(\mathbf{r}_1) \frac{p_i^2}{2m} \psi_i(\mathbf{r}_1) d\mathbf{r}_1 \\ &+ \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N \int \psi_i^*(\mathbf{r}_1) \psi_j^*(\mathbf{r}_2) (\mathbf{r}_{12} | K(\rho) | \mathbf{r}_{12}') \\ &\times [\psi_i(\mathbf{r}_1') \psi_j(\mathbf{r}_2') - \psi_i(\mathbf{r}_2') \psi_j(\mathbf{r}_1')] d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2'. \quad (4) \end{aligned}$$

Following the usual procedure, we now determine the optimum form for W by demanding that W be stationary with respect to variation in the form of the ψ 's, while requiring that the variation procedure preserve the normalization of the wave functions. Varying W of Eq. (4) with respect to $\psi_i^*(\mathbf{r}_3)$, we find

$$\begin{aligned} E_i \psi_i(\mathbf{r}_3) &= \frac{p_i^2}{2m} \psi_i(\mathbf{r}_3) + \sum_{j=1}^N \int \psi_j^*(\mathbf{r}_2) (\mathbf{r}_{23} | K(\rho) | \mathbf{r}_{23}') \\ &\times [\psi_i(\mathbf{r}_3') \psi_j(\mathbf{r}_2') - \psi_i(\mathbf{r}_2') \psi_j(\mathbf{r}_3')] d\mathbf{r}_3' d\mathbf{r}_2 d\mathbf{r}_2' \\ &+ \frac{1}{2} \sum_{i,j=1}^N \int \psi_i^*(\mathbf{r}_1) \psi_j^*(\mathbf{r}_2) \frac{\delta(\mathbf{r}_{12} | K(\rho) | \mathbf{r}_{12}')}{\delta \psi_i^*(\mathbf{r}_3)} \\ &\times [\psi_i(\mathbf{r}_1') \psi_j(\mathbf{r}_2') - \psi_i(\mathbf{r}_2') \psi_j(\mathbf{r}_1')] d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2'. \quad (5) \end{aligned}$$

To evaluate the density variation of the K -matrix appearing in the last term of Eq. (5), we use the relation that

$$\rho(\mathbf{r}) = \sum_i \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}), \quad (6)$$

where the density is to be evaluated at the center of gravity, \mathbf{R} . Thus

$$\frac{\delta(\mathbf{r}_{12} | K(\rho) | \mathbf{r}_{12}')}{\delta \psi_i^*(\mathbf{r})} = \frac{\partial(\mathbf{r}_{12} | K(\rho) | \mathbf{r}_{12}')}{\partial \rho} \frac{\delta \rho(\mathbf{R})}{\delta \psi_i^*(\mathbf{r})}. \quad (7)$$

Substituting Eq. (6) into Eq. (7) and noting that the variation of the density vanishes unless \mathbf{r} coincides

with \mathbf{R} , we find

$$\frac{\delta(\mathbf{r}_{12}|K(\rho)|\mathbf{r}_{12}')}{\delta\psi^*(\mathbf{r})} = \frac{\partial(\mathbf{r}_{12}|K(\rho)|\mathbf{r}_{12}')}{\partial\rho}\psi(\mathbf{r})\delta(\mathbf{R}-\mathbf{r}). \quad (8)$$

Substituting the result of Eq. (8) into Eq. (5), we find the modified Hartree-Fock equation for $\psi_i(\mathbf{r}_3)$ to be

$$E_i\psi_i(\mathbf{r}_3) = \frac{\hbar^2}{2m}\psi_i(\mathbf{r}_3) + \int (\mathbf{r}_3|V|\mathbf{r}_3')\psi_i(\mathbf{r}_3')d\mathbf{r}_3' + V_R(\mathbf{r}_3)\psi_i(\mathbf{r}_3), \quad (9)$$

where

$$(\mathbf{r}_3|V|\mathbf{r}_3') = \sum_j \int \psi_j^*(\mathbf{r}_2)[(\mathbf{r}_{23}|K(\rho)|\mathbf{r}_{23}') - (\mathbf{r}_{23}|K(\rho)|\mathbf{r}_{32}')P_\sigma P_\tau]\psi_j(\mathbf{r}_2)d\mathbf{r}_2d\mathbf{r}_2' \quad (10)$$

is the single particle potential previously defined in I, and

$$V_R(\mathbf{r}_3) = \frac{1}{2} \sum_{jk} \int \psi_j^*(\mathbf{r}_1)\psi_k^*(\mathbf{r}_2) \frac{\partial}{\partial\rho}(\mathbf{r}_{12}|K(\rho)|\mathbf{r}_{12}') \times [\psi_j(\mathbf{r}_1')\psi_k(\mathbf{r}_2') - \psi_j(\mathbf{r}_2')\psi_k(\mathbf{r}_1')] \times \delta(\mathbf{R}-\mathbf{r}_3)d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_1'd\mathbf{r}_2'. \quad (11)$$

This additional potential energy term, V_R , is closely related to the rearrangement energy previously described by one of us (KAB)³ and by Hugenholtz and Van Hove.⁴

The general form for V_R given in Eq. (10) can be considerably simplified if we make use of the density dependence of the K -matrix as determined in I. There it was shown that the variation of K with density could to an excellent approximation be entirely included in the core repulsion part of the K -matrix. According to I,

$$(\mathbf{r}_{12}|K(\rho)|\mathbf{r}_{12}') = (\mathbf{r}_{12}|K|\mathbf{r}_{12}')_{\text{attractive}} + (\mathbf{r}_{12}|K(\rho)|\mathbf{r}_{12}')_{\text{core}}, \quad (12)$$

where $K_{\text{attractive}}$ was independent of ρ and

$$(\mathbf{r}_{12}|K(\rho)|\mathbf{r}_{12}')_{\text{core}} = [A(\rho)/4\pi r_c^2] \times \delta(r_{12}r_c)_{\text{core}}\delta(r_{12}'-r_c), \quad (13)$$

with the constants

$$A_s(\rho) = 215 \times 10^{-13} \text{ Mev-cm} \left(\frac{0.544}{1-0.488/r_0} \right), \text{ singlet}$$

and

$$A_t(\rho) = 257 \times 10^{-13} \text{ Mev-cm} \left(\frac{0.572}{1-0.459/r_0} \right), \text{ triplet} \quad (14)$$

where r_0 is measured in units of 10^{-13} cm. In Eq. (14), the spacing parameter r_0 is related to ρ by the equation

$$\rho^{-1} = (4/3)\pi r_0^3, \quad (15)$$

and r_c is the radius of the hard-core potential.

The very short range of the nonlocality in K_{core} allows simplification of Eq. (11) for V_R , since only relative

³ K. A. Brueckner, Phys. Rev. **110**, 597 (1958).

⁴ N. M. Hugenholtz and L. Van Hove, Physica **24**, 363 (1958).

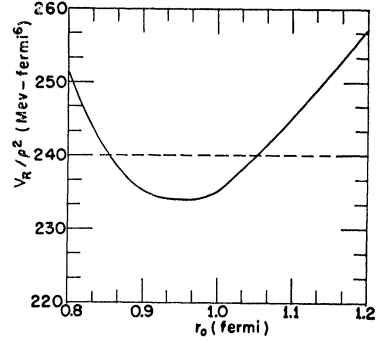


FIG. 1. The ratio of the rearrangement energy, V_R , to the density ρ^2 plotted as a function of the spacing parameter, r_0 .

s -states of particle motion can enter, and also since we can to an excellent approximation set $\mathbf{r}_1' = \mathbf{r}_2' = \mathbf{r}_3$. If we neglect spin or isotopic spin polarization, we then find

$$V_R(\mathbf{r}_3) = \frac{3}{16} \frac{\partial}{\partial\rho} [A_s(\rho) + A_t(\rho)] r_3 4\pi r_c^2 \rho^2(r_3). \quad (16)$$

From Eq. (14) and Eq. (15), we can finally evaluate the density derivatives. The resulting expression for V_R is

$$V_R = \frac{3}{16} \frac{r_c^2}{r_0^3} \left[\frac{117b_s/r_0}{(1-b_s/r_0)^2} + \frac{147b_t/r_0}{(1-b_t/r_0)^2} \right] \text{Mev} \times (10^{-13} \text{ cm}), \quad (17)$$

where $b_s = 0.488$ and $b_t = 0.459$.

In Fig. 1 we have plotted V_R/ρ^2 as a function of r_0 . The variation of this function is very slow, so that to a sufficient approximation we can take

$$V_R = (240 \text{ Mev})\rho^2 \times (10^{-13} \text{ cm})^6.$$

We note that the rearrangement potential V_R does not appear directly in the total energy E , determined from the optimized wave functions ψ_i which are inserted into Eq. (4). The effect on the energy enters only indirectly through the alteration of the wave functions.⁵ A much more interesting effect, of direct physical interest, is on the single-particle eigenvalues. The inclusion of the rearrangement potential allows direct identification of the energy eigenvalue of the most weakly bound particle as the energy required to remove the particle and leave the system in its lowest state.

In conclusion, we have seen that it is possible to modify the Hartree-Fock method used to determine the characteristics of finite nuclei, and thus to include the rearrangement effects. Furthermore we have expressed the rearrangement potential as a simple, though approximate, function of the nuclear density. This modified method is presently being incorporated into computational procedures for treating finite nuclei.⁶

⁵ It might be pointed out here that for the case of nuclear matter, the wave functions are plane waves and hence the total energy does not depend on the rearrangement terms evaluated in the approximation of Eq. (16).

⁶ Brueckner, Lockett, and Rotenberg, Bull. Am. Phys. Soc. Ser. II, **4**, 156 (1959); and to be published.