

so that $\psi_{L^+}(\mathbf{p})$ and $\psi_{s^+}(\mathbf{p})$ can be interpreted as the large and small components of $\psi^+(\mathbf{p})$.

We can now write $\psi^+(\mathbf{p})$ in terms of $\psi_{L^+}(\mathbf{p})$ as

$$\psi^+(\mathbf{p}) = C \begin{bmatrix} \psi_{L^+}(\mathbf{p}) \\ (\boldsymbol{\sigma} \cdot \mathbf{p}) \\ \kappa + p_0 \end{bmatrix} \psi_{L^+}(\mathbf{p}). \quad (\text{A.5})$$

By choosing C in such a way that $\psi^+(\mathbf{p})$ and $\psi_{L^+}(\mathbf{p})$ satisfy the normalization condition

$$\psi^{*-}(\mathbf{p})\psi^+(\mathbf{p}) = \psi_{L^+}^{*-}(\mathbf{p})\psi_{L^+}^+(\mathbf{p}), \quad (\text{A.6})$$

we find

$$C = \left(\frac{\kappa + p_0}{2p_0} \right)^{\frac{1}{2}}, \quad (\text{A.7})$$

$$\psi^+(\mathbf{p}) = \left(\frac{\kappa + p_0}{2p_0} \right)^{\frac{1}{2}} \begin{bmatrix} \psi_{L^+}(\mathbf{p}) \\ (\boldsymbol{\sigma} \cdot \mathbf{p}) \\ \kappa + p_0 \end{bmatrix} \psi_{L^+}(\mathbf{p}). \quad (\text{A.8})$$

By using (A.1), (A.8), and the commutation relation

$$(\boldsymbol{\sigma} \cdot \mathbf{A})(\boldsymbol{\sigma} \cdot \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} + i\boldsymbol{\sigma} \cdot (\mathbf{A} \times \mathbf{B}), \quad (\text{A.9})$$

we can always obtain a result of the form

$$\psi^{*-}(\mathbf{p}')O\psi^+(\mathbf{p}) = \psi_{L^+}^{*-}(\mathbf{p}')[a + b_i\sigma_i]\psi_{L^+}^+(\mathbf{p}), \quad (\text{A.10})$$

where O is a product of the Dirac matrices, and a and b_i are numbers.

Fermi-Thomas Type Approximation for Nuclei

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The Hartree-Fock to Fermi-Thomas reduction is carried through for finite nuclei, starting with the K -matrix formulation. The resulting expression represents the nuclear energy to good accuracy in terms of the density and its first derivatives only; it differs in detail from the semiempirical expressions previously proposed for this purpose. This improved expression shows the inadequacy of the "semi-infinite" approximation used often in earlier studies.

1. INTRODUCTION

IT is well known that a Hartree-Fock like energy expression for a many-fermion system can always be converted to a form depending only on the density and its derivatives. On minimizing such an expression with respect to variations, one obtains a Fermi-Thomas type equation for the density. For problems involving many electrons, this situation has been well explored. In general, however, it is not immediately clear just how rapidly the procedure converges, or whether the resulting expression will be simple enough to be handled by a reasonable amount of labor.

In this work, we report upon a reduction of a Hartree-Fock to Fermi-Thomas type equation for finite nuclei and some of its applications. The Hartree-Fock type basis in this case is provided by the K -matrix theory of Brueckner and collaborators,^{1,2} and in the resulting expression, terms up to $(\nabla\rho)^2$ provide a good approxima-

tion for the energy density. In obtaining this result (Sec. 2), we have used an approximate form of the K matrix, which is substantially nonlocal, in conjunction with a square-well potential. Very probably, this overestimates the neglected higher-derivative terms, which are a measure of nonlocality.

Having thus established the unimportance of higher-derivative terms, we go on to calculate a form of energy density, up to terms in $(\nabla\rho)^2$, which is independent of these approximations. In fact, this form of energy-density is as good as may be profitably extracted from the best currently available K matrices.

It is important for the present applications that the density dependence of the K matrix be accurately known. In the published literature,^{1,2} the K matrices are given numerically as functions of r and r' for a fixed density. Their density dependence is given in an approximate formula¹ expected to be valid roughly for $\rho = 3\rho_0$ to $\rho_0/3$, where ρ_0 is the equilibrium density of nuclear matter. In view of this and the doubts recently raised³ concerning the Gammel-Thaler potentials, which form the basis of BGW K matrices, we do not consider

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¹ K. A. Brueckner, J. L. Gammel, and H. Weitzner, Phys. Rev. **110**, 431 (1958), referred to as BGW in the text. K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961).

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

³ G. Derrick, D. Mustard, and J. M. Blatt, Phys. Rev. Letters, **6**, 69 (1961).

it worthwhile at present to make any calculation more detailed than the ones reported in the following. Nonetheless, it is sufficiently clear, even at this stage, that the procedure described below should be applicable to the nuclear case; and more detailed calculations can be made as soon as the question of interactions is settled and better K matrices become available.

Although the possibility of such a procedure was noted earlier,⁴ the forms of the energy density actually used⁴⁻⁶ for computations have been completely arbitrary. The present method differs significantly from these inasmuch as the form of energy density is, for the first time, uniquely determined from the K -matrix theory and is thus provided with as sound a theoretical basis as is possible in the present state of nuclear theory.

Details of the methods of solving the density equations have been given by Wilets.^{5,6} The use of the "semi-infinite" approximation with our form of energy density does not give a correct falloff distance, which suggests that the success of this approximation in earlier studies must have been due to erroneous forms for the energy expression. In solving the equations without the semi-infinite approximation, we give an improved treatment of the boundary conditions.

As suggestions for further work, we note the possibility of including the second-order effects by a perturbation calculation. The restriction to central densities may be eliminated by converting Eq. (15) into a series of coupled equations for $\rho_{l,m}$ by writing $\rho = \sum_{l,m} \rho_{l,m} V_{l,m}$. This series may be cut off at $\rho_{2,m}$ in view of the unimportance of the higher order multipoles, and solved approximately. Finally, information on the shell-structure itself may be obtained by calculating the distribution of nucleons in various l levels following the well-known Fermi method.

2. THE FORM OF ENERGY DENSITY

The interaction energy according to the K -matrix theory may be written as

$$\Delta E = \Delta E_{nn} + \Delta E_{pp} + \Delta E_{pn}, \quad (1)$$

with

$$\Delta E_{nn} = \frac{1}{4} \sum_{n_i n_j} \int \phi_{n_i}^*(1) \phi_{n_j}^*(2) K_{s,e}(12, 1'2') \times \phi_{n_i}(1') \phi_{n_j}(2') d1 d2 d1' d2', \quad (2a)$$

$$\Delta E_{pp} = \frac{1}{4} \sum_{p_i p_j} \int \phi_{p_i}^*(1) \phi_{p_j}^*(2) K_{s,e}(12, 1'2') \times \phi_{p_i}(1') \phi_{p_j}(2') d1 d2 d1' d2', \quad (2b)$$

$$\Delta E_{pn} = \sum_{p_i n_j} \phi_{p_i}^*(1) \phi_{n_j}^*(2) \left(\frac{1}{4} K_{s,e} + \frac{3}{4} K_{t,e} \right) \times \phi_{p_i}(1') \phi_{n_j}(2') d1 d2 d1' d2', \quad (2c)$$

where ϕ 's are the single-particle wave functions in the

model potential, and the subscripts s, e and t, e denote the singlet-even and triplet-even parts.¹ By expanding each wave function pair $\phi_i(r_1)\phi_j(r_2)$ about the center of mass, one can express ΔE in terms of the densities

$$\rho_n(R) = \sum_i |\phi_{n_i}(R)|^2, \quad \rho_p(R) = \sum_i |\phi_{p_i}(R)|^2, \quad \rho_n + \rho_p = \rho, \quad (3)$$

and their derivatives.

To show that only the terms up to the first derivatives are important, we take the approximate form of the K matrix given by BGW¹ for the singlet s state:

$$\langle \mathbf{r}_1 \mathbf{r}_2 | K | \mathbf{r}_1' \mathbf{r}_2' \rangle = \delta(\mathbf{R} - \mathbf{R}') \left\{ -\frac{\delta(r' - r_c) \delta(r - r_c)}{(4\pi r_c^2)^2 G_0(r_c, r_c)} - \left[\frac{\delta(r - r_c)}{4\pi r_c^2} v_a(r') \frac{G_0(r', r_c)}{G_0(r_c, r_c)} + r' \leftrightarrow r \right] + v_a(r) \frac{\delta(r - r')}{4\pi r^2} \right\}, \quad (4)$$

where \mathbf{R} and \mathbf{r} are the center-of-mass and relative coordinates, respectively, r_c is the core radius, v_a is the attractive part of the potential in question, and G_0 is the s -state Green's function given approximately by²

$$G_0(r, r') \approx \frac{1}{rr'} \exp \left[-\frac{\alpha}{\hbar} |r - r'| \right] - \exp \left[-\frac{\alpha}{\hbar} (r + r') \right]; \quad \frac{\hbar}{\alpha} = 1.07 \text{ f.} \quad (5)$$

The K matrix for the triplet state has the same form if we assume that only the s -state interactions are important.

We use this form of the K matrix for its simplicity and because it has substantial nonlocality. The derivative terms are a measure of the nonlocality of the interaction, and it seems that in conjunction with a square-well potential this form overestimates the effects of nonlocality and, hence, the derivative terms. If we form the quantity¹ $f(r) = \int (\mathbf{r} | K | \mathbf{r}') d\mathbf{r}'$, then a measure of nonlocality is given by the distance at which $f(r)$ becomes indistinguishable from $v(r)$. With quantities mentioned above and a hard core radius $r_c = 0.4$ f, $f(r)$ is 79% of $v(r)$ at $r = 1$ f and 92% at 1.5 f.

Putting, for simplicity,

$$2\rho_n(R) = 2\rho_p(R) = \rho(R), \quad (6a)$$

and

$$(r_c)_t = (r_c)_s, \quad (6b)$$

and assuming interactions only in the s state, we have after some manipulations with (1), (2), and (4) for the energy density:

$$\mathcal{E}(\rho) = c\rho^{5/3} - a_1\rho^2 + a_2(\nabla\rho)^2 + \frac{4}{3}a_2\tau\rho, \quad (7)$$

⁴ T. H. R. Skyrme, Phil. Mag. **1**, 1043 (1956).

⁵ R. A. Berg and L. Wilets, Phys. Rev. **101**, 201 (1956).

⁶ L. Wilets, Phys. Rev. **101**, 1805 (1956), and Revs. Modern Phys. **30**, 542 (1958).

where

$$c = 3.6\hbar^2/2M, \quad \tau = \sum_i |\nabla\phi_i|^2 \cong 3.6\rho^{\frac{5}{3}}, \quad (8a)$$

$$-a_1 = \frac{3}{16} \left\{ \left[\int v(r) \left(1 - 2 \frac{G_0(r, r_c)}{G_0(r_c, r_c)} \right) d^3r \right] - \frac{4}{G_0(r_c, r_c)} \right\}, \quad (8b)$$

$$-a_2 = \frac{3}{128} \left\{ \left[\int v(r) \left(r^2 - (r^2 + r_c^2) \frac{G_0(r, r_c)}{G_0(r_c, r_c)} \right) d^3r \right] - \frac{4r_c^2}{G(r_c, r_c)} \right\}, \quad (8c)$$

$$v = v_{a,s} + v_{a,t}. \quad (8d)$$

The main point we wish to make is that the corrections to Eq. (7) are very small. The largest of these corrections arise from the second and third terms in Eq. (4), and their smallness can be traced to the rapid damping inside the relevant integrals caused by the Green's function. This rapid damping is a characteristic of the Green's function, and we do not expect likely refinements on Eq. (5) to change the magnitudes appreciably. Explicit calculations were made up to the terms involving the fourth derivatives of the density. We shall not give the details of these calculations, which are straightforward, if tedious. The magnitudes of the main term and the corrections were estimated at various values of the density for a Saxon-Wood type distribution, Eq. (9), and the approximate form of the Green's function given in Eq. (5) was used.

$$\rho = \rho_0 \frac{1}{1 + e^{x/a}}; \quad \rho_0 = 0.2 \text{ f}^{-3}; \quad x = (r - R); \quad a = 0.5 \text{ f}. \quad (9)$$

A quantity $\theta = \sum_i |\nabla^2\phi_i|^2 \cong 16\rho^{7/3}$ was also needed. The potential was assumed to be a square well of depth 30 Mev and range 2 f with a hard core at 0.4 f. There appear some systematic cancellations, and the magnitude of the corrections at their highest was about 6% of the main terms displayed in Eq. (7). The magnitude of the corrections depends on the range of the potential and the hard core but not on its depth.

Energy expressions similar to that in Eq. (7) have been discussed by many authors, notably by Skyrme,⁴ Berg and Wilets,⁵ and Wilets,⁶ who also show the connection with surface phenomena. The chief difference is that they either assume a simple form for $\mathcal{E}(\rho)$ or leave it unspecified. Choosing a so-called phenomenological or semiempirical form of $\mathcal{E}(\rho)$ is equivalent to assuming some arbitrary form for a_1 and a_2 . However, the expressions in Eq. (8) result directly from the K -matrix theory. Of course, they depend on the particular form (4) of the K matrix, but more general relations can be

easily written down. An approximate density dependence of a_1 and a_2 , independent of the form (5) of the Green's function, may be obtained by using a relation given by Brueckner *et al.*¹:

$$K(\rho) = K_{\text{core}}(\rho) + K_a, \quad (10a)$$

$$K_{\text{core}}(\rho) = K_{\text{core}}(\rho_0)f(\rho); \quad f(\rho) = 0.58/(1 - 0.78\rho^{\frac{1}{3}}). \quad (10b)$$

The density dependence of the K operator in singlet and triplet states differs only slightly. We have written for simplicity, $f_s = f_t = f$. Hence,

$$a_1(\rho) = b_1 + d_1 f(\rho), \quad (11a)$$

$$a_2(\rho) = b_2 + d_2 f(\rho), \quad (11b)$$

where

$$b_1 = \frac{3}{16} \int v(r) d^3r, \quad b_2 = \frac{3}{128} \int r^2 v(r) d^3r. \quad (12)$$

The form (4) of the K matrix is obtained by using the Born approximation for the perturbed wave function outside the core radius. It may be verified¹ that higher-order corrections will bring in only density-dependent corrections. Hence, the density-independent parts are given correctly by (12). Since we have taken the density-dependent part from the analysis of BGW,¹ we have, in Eq. (11), as good a representation of these quantities as can be obtained in the present state of the K -matrix theory. It might be remarked that a straightforward use of Eq. (5) in (8) gives incorrect density dependence of a_1 and a_2 , as might be expected.

For Gammel-Thaler potentials quoted by BGW,¹ $b_1 = 476 \text{ Mev f}^3$, $b_2 = 158 \text{ Mev f}^5$. By requiring that the equilibrium density of nuclear matter be $\rho_0 = 0.2 \text{ f}^{-3}$ and the binding energy per particle at the minimum be 15 Mev, we obtain $d_1 = -90 \text{ Mev f}^3$, $d_2 = -47 \text{ Mev f}^5$. This gives $a_2(\rho_0) \cong 108 \text{ Mev f}^5$, which corresponds to an effective mass of 0.4 for nuclear matter. These values show that the density dependences of a_1 and a_2 are given nearly correctly by (11), at least for densities close to the nuclear densities. For densities which are much higher or much lower, the behavior of a_1 and a_2 may not be well represented in this way—as is the case with the underlying K -matrix theory itself.

3. APPLICATION TO NUCLEI

In applying Eq. (7) to finite nuclei, we require that the total energy be minimum with respect to variation of the density under the constraint of a given number A of particles. That is,

$$\delta \int [\mathcal{E}(\rho) - \lambda' \rho] d^3r = 0, \quad (13)$$

where λ' is the Lagrange parameter to be determined from the condition that

$$A = \int \rho d^3r. \quad (14)$$

A nonlinear differential equation is thus obtained. Neglecting the density dependence of a_1 and a_2 , it is

$$\nabla^2 y = 0.993y^3 + 2.15y^{5/3} - 3.417y + \lambda, \quad (15)$$

where $y = \rho/\rho_0$ and the values of constants derived earlier have been used.

In the semi-infinite approximation,⁴⁻⁶ one puts $\nabla^2 = d^2/dr^2$. This amounts to neglecting the effect of the $(2/r)d/dr$ term, and was made plausible by arguing that the derivative is important only in the surface where the large value of r will make the term negligible. In this approximation, the boundary conditions $dy/dr = 0$ at both $y = 1$ and $y = 0$ uniquely fix $\lambda = 0.304$. The 90–100% falloff distance for y turns out to be 3.3 f. This is to be compared with the experimental value quoted to be between 2.2 and 2.5 f.

The semi-infinite approximation is removed by taking the full expression $\nabla^2 = d^2/dr^2 + (2/r)d/dr$ in (15). The origin of coordinates assumes special significance here, and it is no longer possible to fix λ as before. We require solutions of (15) which have the correct density profile for which $y \rightarrow 1$ as $r \rightarrow 0$ and $y \rightarrow 0$ as $r \rightarrow \infty$. In actual practice, one has to make a choice of λ and a boundary value till the right solution is obtained. The area under the curve determines the value of A which thus depends on λ and the boundary value from which the integration of the equation was started.

One here comes across a difficulty of principle obscured by the semi-infinite approximation, inasmuch as the present method, like the Fermi-Thomas method, breaks down at small values of density. The density for large values of r should decay exponentially. This does not seem to be the property of the solutions of Eq. (15). Connection of Fermi-Thomas method to the WKB approximation has been discussed by many authors and suggests that the method breaks down at the classical turning points for particles moving in a potential. The exact value of density for which the present expression breaks down will also depend on the K -matrix expression in a manner which, at the moment, can not be determined. In view of this, we match the solution at a large enough value of r to an exponential $e^{-2\epsilon r}$, where

$\epsilon^2 = \hbar^2|E|/2m$, E being the binding energy of the last particle whose contribution to the density is the most important one at large distances. λ in (13) is the chemical potential and is therefore connected to E . Still, there is considerable arbitrariness in the choice of boundary values, although this procedure answers a question of principle.

With the same parameters as before (neglecting the density dependence of a_1 and a_2), a double eigenvalue search, in the manner indicated, yields a falloff distance of about 4 f. To obtain the correct value one needs considerably stronger potentials. However, for a wide variation of parameters the falloff distances obtained in this way are 0.5 to 0.7 f larger than the ones obtained in the semi-infinite approximation—thus showing the inadequacy of the latter. In this connection we also propose to examine the full differential equation incorporating the density dependence of a_1 and a_2 instead of Eq. (15).

4. CONCLUSIONS

We have shown that, if the basic assumptions of the BGW method are granted, then, one can set up a simple Fermi-Thomas type of equation for studying various nuclear properties. We have indicated how the accuracy of such a calculation might be determined, and have derived a form of energy density which is correct to about 6%. Application to density distributions shows the inadequacy of certain approximations.

It does not seem very profitable at this moment to make any more detailed calculations because of the doubts recently raised concerning the Gammel-Thaler potentials,³ and because of the limited range of validity of the published form of the K -matrix density dependence. Suggestions for further work are included in the introduction.

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