Application of the Reference-Spectrum Method to the Nuclear Surface*†

B. D. DAY
University of California, Los Angeles
(Received 1 July 1964)

The reference-spectrum method for infinite nuclear matter is generalized in a simple way so as to apply to the surface region of a large nucleus. This permits one to calculate the reaction matrix for particles interacting in the surface region, and the total energy of the nucleus can therefore be found to first order in the Brueckner-Goldstone expansion. Two equivalent formulas for the nuclear surface energy, both valid to first order in the Brueckner-Goldstone expansion, are derived and discussed. These results are then used to calculate the surface energy of a large nuclear slab. The single-particle wave functions are calculated in a Woods-Saxon potential which is chosen to reproduce the empirical surface thickness; and the two-body interaction, which acts only in S states, is assumed to consist of an exponential attraction outside a hard core. The calculation gives the reasonable value of $20.6\,A^{2/3}$ MeV for the surface term in the semiempirical mass formula. The chief defect of this trial calculation is the lack of self-consistency in the one-particle wave functions. A self-consistent calculation would give a more reliable estimate for the surface energy and would also predict the surface thickness theoretically. A brief discussion is given of how the methods of this paper could be used to attack the self-consistency problem.

I. INTRODUCTION

A NUMBER of theoretical investigations of the nuclear surface have been carried out in the past. The phenomenological treatments are typified by the "semiempirical statistical method" developed by Wilets,[1] which allows one to derive relations among various experimental quantities without becoming involved in the full complexity of the many-body problem. Similar methods have been applied by Skyrme,[2] by Bodmer,[3] and by Hale and Present.[4] Swiatecki[5] has considered a plane nuclear surface by means of perturbation theory, and Rotenberg[6] has obtained a reasonable surface thickness in his Hartree-Fock treatment of a finite nucleus. Both of these authors used nonsingular two-body interactions, however. Blanchard and Seyler,[7] in their semiclassical nuclear model, have included the short-range repulsion, which is known to exist between two nucleons, by means of a velocity-dependent force. Their model of finite nuclei has reasonable surface properties. The Green's function approach has been sucessfully applied by Reynolds,[8] using a separable potential with a "hard shell" repulsion. Brueckner, Gammel, and Weitzner[9] have extended Brueckner's nuclear matter theory[10] to the case of finite nuclei, and calculations have been made on several doubly-magic nuclei.[11] These calculations are certainly the most ambitious and realistic which have been made, but the binding energies and nuclear radii obtained are somewhat too small, especially for the lighter nuclei. Since the theory is specifically designed to be correct for infinite nuclear matter, it seems likely that the surface region is causing the trouble, and further study of the nuclear surface appears to be worthwhile.

Brueckner's theory is based on the Brueckner-Goldstone perturbation series,[12] and the basic quantity in this expansion is the reaction matrix, or G matrix. The development of the reference spectrum method by Bethe, Brandow, and Petschek (BBP)[13] has provided a new and much simpler method of calculating the nuclear matter G matrix than was previously available. It is therefore worthwhile to see if this method can be applied to the nuclear surface, and the present work makes a start in this direction. We first generalize the reference-spectrum method in a simple way so that it may be used in the surface region. It is found that the G matrix may be easily calculated, once the two-body wave function is obtained. The wave equation for this function is derived, and two methods for its solution are discussed. It is also necessary to obtain, within the framework of the Brueckner-Goldstone theory, a formula for the surface energy, and two such formulas are derived. The method is finally used for a numerical trial calculation of the nuclear surface energy.

* Supported in part by the U. S. National Science Foundation, and by the U. S. Office of Naval Research.
† Based in part on a thesis submitted to Cornell University for the Ph.D. degree.
[1] L. Wilets, Rev. Mod. Phys. **30**, 543 (1958); R. A. Berg and L. Wilets, Phys. Rev. **101**, 201 (1956); L. Wilets, Phys. Rev. **101**, 1805 (1956).
[2] T. H. R. Skyrme, Phil. Mag. **1**, 1043 (1956).
[3] A. R. Bodmer, Nucl. Phys. **17**, 388 (1960).
[4] D. P. Hale and R. D. Present, Phys. Rev. **104**, 448 (1956).
[5] W. J. Swiatecki, Proc. Phys. Soc. (London) **A64**, 226 (1951); Phys. Rev. **98**, 203 (1955); Proc. Phys. Soc. (London) **A68**, 285 (1955).
[6] M. Rotenberg, Phys. Rev. **100**, 439 (1955).
[7] R. G. Seyler and C. H. Blanchard, Phys. Rev. **124**, 227 (1961); Phys. Rev. **131**, 355 (1963).
[8] J. C. Reynolds, Phys. Rev. **130**, 1891 (1963).
[9] K. A. Brueckner, J. L. Gammel, and H. Weitzner, Phys. Rev. **110**, 431 (1958); see also K. A. Brueckner and D. T. Goldman, Phys. Rev. **116**, 424 (1959).
[10] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).
[11] K. A. Brueckner, A. M. Lockett, and M. Rotenberg, Phys. Rev. **121**, 255 (1961); K. S. Masterson and A. M. Lockett, Phys. Rev. **129**, 776 (1963).
[12] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).
[13] H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963). This paper will hereafter be referred to as BBP.

II. GENERALIZATION OF THE REFERENCE SPECTRUM METHOD

To apply the Brueckner-Goldstone theory,[12] one starts with a single-particle Hamiltonian h which has a complete orthonormal set of eigenfunctions $\phi_n(\mathbf{r})$ with eigenvalues ϵ_n, i.e. $h(\mathbf{r})\phi_n(\mathbf{r})=\epsilon_n\phi_n(\mathbf{r})$. If the nucleus under consideration contains A particles, the unperturbed many-body ground state is formed by putting particles into the A one-particle states of lowest energy to form a Slater determinant. These normally occupied states make up what is called the Fermi sea, while one-particle states of higher energy are called intermediate states. One must then compute matrix elements of the two-body operator G, which is defined by

$$G=v-v(Q/e)G. \tag{2.1}$$

Here, v is the two-body potential, Q is the Pauli operator which prohibits scattering into occupied states, and e is an operator whose coordinate space representation is

$$e(\mathbf{r}_1,\mathbf{r}_2)=h(\mathbf{r}_1)+h(\mathbf{r}_2)-H, \tag{2.2}$$

where H is the starting energy.[14] The first-order approximation to the ground-state energy is

$$E\approx\sum_n\langle n|T|n\rangle+\tfrac{1}{2}\sum_{mn}\langle mn|G|mn-nm\rangle, \tag{2.3}$$

where T is the kinetic energy. Of course, if this is to be a good approximation, the ϕ_n's and ϵ_n's must be chosen self-consistently. We assume for the moment that this difficult task has somehow been accomplished and turn our attention to the problem of calculating matrix elements of G.

For the interaction of two particles in states ϕ_m and ϕ_n, the unperturbed two-particle wave function $\Phi_{mn}(\mathbf{r}_1,\mathbf{r}_2)$ is just the product of $\phi_m(\mathbf{r}_1)$ and $\phi_n(\mathbf{r}_2)$, and we define the exact two-body wave function $\Psi_{mn}(\mathbf{r}_1,\mathbf{r}_2)$ by

$$G\Phi_{mn}(\mathbf{r}_1,\mathbf{r}_2)=v\Psi_{mn}(\mathbf{r}_1,\mathbf{r}_2). \tag{2.4}$$

When $r\equiv|\mathbf{r}_1-\mathbf{r}_2|$ becomes large, Ψ_{mn} must approach Φ_{mn}, and if v contains a hard core, Ψ_{mn} must vanish whenever $r\leq c$, where c is the core radius. Combining (2.1) and (2.4) leads to

$$\Psi_{mn}=\Phi_{mn}-(1/e)Qv\Psi_{mn}, \tag{2.5}$$

which is a difficult equation to solve because of the presence of the rather complicated operator Q/e.

The basic idea of the reference-spectrum method is to approximate Q/e by a simpler operator. Then (2.5) can be easily solved, and the small error caused by the approximation can be calculated by a perturbation method.[15] For the problem of nuclear matter, BBP have shown that, for the purpose of operating on states with momenta in the "important range" between 3 and 5 inverse fermis (F^{-1}), h can be well approximated by the "reference Hamiltonian" h^R, given by

$$h^R=-(1/2m^*)\nabla^2+A_2. \tag{2.6}$$

In this equation, m^* is the dimensionless effective mass,[16] which BBP estimate to be about 0.9, and A_2 is a constant which seems from the work of BBP to be very close to zero. It is not a good approximation to replace h by h^R when operating a state whose momentum is outside the range 3 F^{-1} to 5 F^{-1}, but the Fourier components of the function $Qv\Psi_{mn}$, to which the operator e^{-1} is applied in (2.5), are small outside this momentum range. It is thus quite accurate in (2.5) to replace e by e^R, where e^R is defined by (2.2) with h replaced by h^R. Having set e equal to e^R in (2.5), we may replace Q by unity without causing serious error because $1/e^R$ applied to states in the Fermi sea gives a rather small result. These approximations are discussed quantitatively in BBP, where it is estimated that they cause an error of about 5% in the potential energy per particle of nuclear matter.

When Q/e is replaced by $1/e^R$, (2.5) becomes

$$e^RZ_{mn}=v\Psi_{mn}, \tag{2.7}$$

where we have defined $Z_{mn}=\Phi_{mn}-\Psi_{mn}$. In infinite nuclear matter the one-particle wave functions are just plane waves, e.g., $\phi_m(\mathbf{r}_1)=\Omega^{-1/2}e^{i\mathbf{k}\cdot\mathbf{r}_1}$, where Ω is the normalization volume. So, by putting (2.6) into (2.2) to find e^R, and changing to relative and center-of-mass coordinates via the equations

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2, \qquad \mathbf{k}=\tfrac{1}{2}(\mathbf{k}_m-\mathbf{k}_n), \tag{2.8}$$

$$\mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2), \quad \mathbf{K}=\mathbf{k}_m+\mathbf{k}_n, \tag{2.9}$$

we find that (2.7) becomes

$$[\nabla_r^2-\gamma^2]\zeta_{mn}(\mathbf{r})=-m^*v\psi_{mn}(\mathbf{r}), \tag{2.10}$$

which is the reference wave equation of BBP and is easily solved by standard methods. In this equation, γ^2 is given by

$$\gamma^2=\tfrac{1}{4}K^2+m^*(2A_2-H), \tag{2.11}$$

and the center-of-mass motion has been eliminated by writing

$$\begin{pmatrix}\Psi_{mn}\\ \Phi_{mn}\\ Z_{mn}\end{pmatrix}=\Omega^{-1}\exp(i\mathbf{K}\cdot\mathbf{R})\begin{pmatrix}\psi_{mn}(\mathbf{r})\\ \phi_{mn}(\mathbf{r})\\ \zeta_{mn}(\mathbf{r})\end{pmatrix}, \tag{2.12}$$

where $\phi_{mn}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}$, and $\zeta_{mn}=\phi_{mn}-\psi_{mn}$.

These ideas can now be applied to a nucleus with a surface. The only difference is that the one-particle Hamiltonian h will change as we pass through the surface region, and our reference approximation h^R for this operator must vary in a corresponding way.

Let us consider a large nuclear slab of thickness L and

[14] The proper choice of H is discussed in detail in BBP. For our purposes, it will always be correct to set $H=\epsilon_m+\epsilon_n$, where m and n label the initial states of the two interacting particles.

[15] This correction is considered in BBP but will be neglected here.

[16] We use units in which $\hbar^2M^{-1}=1$, where M is the nucleon mass. Energy is then measured in inverse square fermis, and this can be converted into MeV by using the relation 1 $F^{-2}=41.467$ MeV.

area $\mathcal{A}$. We will eventually allow $\mathcal{A}$ and L to become infinite in such a way that $L\mathcal{A}^{-1/2}$ goes to zero; thus the surface area becomes equal to $2\mathcal{A}$ in the limit. We take the x axis normal to the surface of area $\mathcal{A}$ and let the nucleus extend from $x=0$ to $x=-L$. We essentially have translational invariance in directions perpendicular to the x axis, and the one-particle wave functions are therefore of the form

$$\phi_n(\mathbf{r})=2^{1/2}N_n^{-1/2}\mathcal{A}^{-1/2}\exp(i\mathbf{k}_{n\perp}\cdot\mathbf{r}_\perp)u_n(x), \quad (2.13)$$

where, for occupied states, $u_n(x)$ decays exponentially outside the nucleus and becomes a sine wave of unit amplitude inside. N_n is a normalization constant which is approximately equal to L, and the subscript "$\perp$" is used to indicate that part of any vector which is normal to the x axis.

Far inside the nucleus, conditions are the same as in nuclear matter, and h^R must be given by (2.6). Far outside, we just have empty space, and h^R must reduce to $-\frac{1}{2}\nabla^2$, the correct result for free particles. In either of the two surface regions, near $x=0$ or $x=-L$, h^R must vary smoothly from its nuclear matter value to its free-space value. The simplest operator which has this property is

$$-\frac{1}{2m^*}f(x)\nabla^2-\frac{1}{2m^*}\frac{df}{dx}\frac{\partial}{\partial x}+A_2w(x), \quad (2.14)$$

where $f(x)$ approaches 1 inside the nucleus and m^* outside, and $w(x)$ goes from a value of 1 inside to zero outside. The term involving (df/dx), which is necessary in order that the operator be Hermitian, is nonzero only in the surface region.

The behavior of $f(x)$ and $w(x)$ must be adjusted in the surface region to make the effect of (2.14) on the important intermediate states very nearly the same as the effect of h on these states. Assuming that this can be done, we use (2.14) for h^R and substitute into (2.7) to obtain the approximate equation

$$\left\{-\frac{1}{2m^*}\left[\nabla_1^2+\nabla_2^2+\frac{df(x_1)}{dx_1}\frac{\partial}{\partial x_1}+\frac{df(x_2)}{dx_1}\frac{\partial}{\partial x_2}\right]+A_2[w(x_1)+w(x_2)]-H\right\}Z_{mn}(\mathbf{r}_1,\mathbf{r}_2)=v\Psi_{mn}(\mathbf{r}_1,\mathbf{r}_2). \quad (2.15)$$

By solving (2.15) one can obtain an approximation for Ψ_{mn} and hence for the G matrix. The dependence of (2.15) on $\mathbf{R}_\perp$ is trivial, but the dependence on X, the x component of $\mathbf{R}$, is not. Thus, we are faced with a differential equation in which the variables $\mathbf{r}$ and X are thoroughly "mixed together." There is no standard method for solving such an equation, and each case must be treated individually by suitable approximation methods.

The question of whether the self-consistent h can be well represented by (2.14) in the surface region remains open. To investigate this point, it is necessary to decide upon a self-consistency condition for the one-particle potential U, i.e., to decide which higher order diagrams in perturbation theory are to be cancelled by proper choice of this potential.[17,18] This will lead to a prescription for calculating U in terms of matrix elements of G. Hence U can be estimated, and one can see if $f(x)$ and $w(x)$ can be chosen in such a way that (2.14) is a good approximation to $h\equiv T+U$. The methods of this paper could be used for this purpose, but this has not yet been done.

Setting the Pauli operator Q equal to unity should be an even better approximation in the surface region than in nuclear matter. When the particle density becomes low, Q prohibits fewer and fewer intermediate states and has a correspondingly smaller effect on the correct wave function Ψ_{mn}.

In order to calculate the wave functions of occupied states, we can try to represent h by an expression of the same form as (2.14) but with different values of m^* and A_2 and different functions f and w. The effective mass should probably be about 0.6,[10] and A_2 must be negative and of the order of 100 MeV in magnitude. These changes are necessary because we want to approximate the effect of the self-consistent h on normally occupied states, while our previous discussion was concerned with highly excited intermediate states with momenta between 3 F^{-1} and 5 F^{-1}. To see whether or not the effect of h on occupied states can be approximated in this way one must carry out an investigation similar to that outlined above for intermediate states.

III. TRIAL CALCULATION

A. Simplifying Assumptions

We have carried out a trial calculation along the lines suggested above. For simplicity, the following rather drastic assumptions were made.

First, the one-particle potential $U(x)$ for occupied states was taken to be a local Woods-Saxon well, defined by saying that

$$U(x)=-U_0(1+e^{x/a})^{-1}, \quad \text{when} \quad x\geq-\tfrac{1}{2}L \quad (3.1)$$

and that $U(x)$ is symmetric about the point $x=-\frac{1}{2}L$. The constant U_0 is determined by requiring that the energy per particle of nuclear matter, given by $0.3k_F^2-\frac{1}{2}U_0$, be -15 MeV. Taking $k_F=1.5$ F^{-1} then leads to a value for U_0 of 2.07 F^{-2}. The length a was set equal to 0.8 F, and the calculated particle density was then found to have a reasonable "90–10 distance" of

[17] The self-consistency condition for nuclear matter is discussed by BBP and by R. Rajaraman, Phys. Rev. **129**, 265 (1963).

[18] A very careful and detailed investigation of this question for finite nuclei has been made by B. H. Brandow in his Ph.D. thesis, Cornell University, 1964 (unpublished). See also Brandow's note in Phys. Letters 4, 8 (1963).

2.48 F. This potential is unrealistic because it has no velocity dependence, and a better calculation could be made by using a one-particle Hamiltonian of the form given by expression (2.14). The reference Hamiltonian for intermediate states is chosen to be simply

$$h_R=-(2m^*)^{-1}\nabla^2, \tag{3.2}$$

with $m^*=0.9$. This is obtained from (2.14) by setting A_2 equal to zero (in accord with BBP) and $f(x)$ equal to unity. This choice gives the correct result inside the nucleus but fails to reduce to the free-particle Hamiltonian outside. We can hope the resulting error will not be too serious since the two values of h_R differ by only 10%.

The two-body potential is assumed to be that considered previously by Moszkowski and Scott[19] and consists of an exponential attraction outside an infinitely repulsive core. The potential acts only in S states, for which it is given by

$$\begin{aligned} v(r)&=+\infty, && r<c,\\ &=-v_0\exp(-\mu(r-c)), && r>c, \end{aligned} \tag{3.3}$$

where $v_0=6.2737$ F$^{-2}=260$ MeV, $\mu=2.08306$ F^{-1}, and $c=0.4$ F.

On the basis of these assumptions, we have calculated the one-particle wave functions and the diagonal G-matrix elements which appear in the first-order expression for the ground state energy. By comparing the energy of our nuclear slab, which has a surface, to that of infinite nuclear matter, we have obtained an estimate for the nuclear surface energy. Our next task is to derive the formulas which are needed to carry out these calculations.

B. One-Particle Wave Functions

The one-particle wave functions have the form of expression (2.13), and by requiring that this be an eigenfunction of $-\frac{1}{2}\nabla^2-U_0(1+e^{x/a})^{-1}$, we find that the Schrödinger equation for $u_n(x)$ is, for $x>-\frac{1}{2}L$,

$$\frac{d^2u_n}{dx^2}+[k_{nx}{}^2-2U_0(1+e^{-x/a})^{-1}]u_n(x)=0. \tag{3.4}$$

We need only consider the region $x>-\frac{1}{2}L$ in detail because, once the wave functions in this region are known, those in the region $x<-\frac{1}{2}L$ can be found from symmetry considerations. The energy eigenvalue is given by

$$\epsilon_n=\tfrac{1}{2}\mathbf{k}_n{}^2-U_0, \tag{3.5}$$

where $\mathbf{k}_n$ is the vector whose x component is k_{nx} and whose perpendicular component is $\mathbf{k}_{n\perp}$. The wave function $u_n(x)$ is normalized such that

$$u_n(x)\sim-\sin(k_{nx}x+\alpha), \tag{3.6}$$

when x is in the interior of the nucleus, where α is a phase factor which depends on k_{nx}. This phase factor is determined by integrating Eq. (3.4) from far outside the nucleus, where the exponentially decreasing solution must be taken, in towards the interior, and comparing the resulting function with the asymptotic form (3.6).

If one starts far to the right of the nucleus and integrates towards the interior in this way, the resulting wave function must join smoothly, at $x=-\frac{1}{2}L$, with the function obtained by starting far to the left of $x=-L$ and integrating inwards. This condition determines the allowed values of k_x, and one easily finds that these allowed values are determined by the equation

$$\tfrac{1}{2}k_xL-\alpha(k_x)=\tfrac{1}{2}n\pi;\quad n=1,2,3,\cdots. \tag{3.7}$$

C. Calculation of the G Matrix

Since $G\Phi_{mn}=v\Psi_{mn}$, the matrix element $\langle mn|G|mn\rangle$ is just the integral of $\Phi_{mn}{}^*v\Psi_{mn}$. In the case of nuclear matter, we introduce partial waves by writing

$$\begin{pmatrix}\psi_{mn}(\mathbf{r})\\ \phi_{mn}(\mathbf{r})\\ \zeta_{mn}(\mathbf{r})\end{pmatrix}=\sum_{LM} i^L[4\pi(2L+1)]^{1/2}r^{-1}\begin{pmatrix}u_{LM}(r)\\ \phi_{LM}(r)\\ \zeta_{LM}(r)\end{pmatrix}Y_{LM}(\hat{r},\hat{x}), \tag{3.8}$$

where $Y_{LM}(\hat{r},\hat{x})$ is a spherical harmonic of $\mathbf{r}$ taken in a system whose polar axis is in the x direction. Taking the polar axis in the x direction, rather than in the direction of the relative momentum vector, will later prove convenient when the presence of the nuclear surface is taken into account. Since $\phi_{mn}(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})$, we find that

$$\phi_{LM}(r)=\left[\frac{(L-|M|)!}{(L+|M|)!}\right]^{1/2}P_{LM}(\hat{k}\cdot\hat{x})rj_L(kr), \tag{3.9}$$

where $\mathbf{k}_\perp$ has been taken to point in the direction whose azimuthal angle φ is zero.

In terms of partial waves, we easily find for the nuclear matter G matrix,

$$\langle mn|G|mn\rangle=\Omega^{-1}\sum_{LM}4\pi(2L+1)\times\int_0^\infty\phi_{LM}(r)v(r)u_{LM}(r)dr. \tag{3.10}$$

This result cannot be used in its present form for a potential with a hard core, but BBP have shown how to derive a useful expression for the radial integral. We shall later have to evaluate a radial integral which differs from (3.10) in that $u_{LM}(r)$ corresponds to k_0, γ^2, while $\phi_{LM}(r)$ is the free wave function for a different pair of parameters, say k, ω^2. Rajaraman,[17] using the methods of BBP, has shown that this more general radial integral

[19] S. A. Moszkowski and B. L. Scott, Ann. Phys. (N. Y.) 11, 65 (1960).

is given by

$$\int_0^\infty \phi_{LM}(k,r)v(r)u_{LM}(k_0,\gamma,r)dr=\frac{\gamma^2+k^2}{m^*}\int_0^c \phi_{LM}(k,r)\phi_{LM}(k_0,\gamma,r)dr+\frac{1}{m^*}\phi_{LM}(k_0,c)\left[\frac{d\phi_{LM}(k,r)}{dr}-\frac{dH_{LM}(k,r)}{dr}\right]_{r=c}$$
$$+\int_c^\infty [\phi_{LM}(k,r)-H_{LM}(k,r)]vu_{LM}(k_0,\gamma,r)dr, \quad (3.11)$$

where H_{LM} is defined by

$$H_{LM}(k,r)=\phi_{LM}(k,c)h_L^{(1)}(i\gamma r)/h_L^{(1)}(i\gamma c). \quad (3.12)$$

By setting $k=k_0$ in (3.11), one obtains the BBP formula for the radial integral of (3.10).

For the problem of the nuclear slab, we have seen that the dependence of the two-particle wave functions on $\mathbf{R}_\perp$ is trivial, while their dependence on X and $\mathbf{r}$ is not. This fact motivates us to write

$$\begin{pmatrix}\Psi_{mn}(\mathbf{r}_1,\mathbf{r}_2)\\ \Phi_{mn}(\mathbf{r}_1,\mathbf{r}_2)\\ Z_{mn}(\mathbf{r}_1,\mathbf{r}_2)\end{pmatrix}=\frac{2}{\mathcal{A}N_m^{1/2}N_n^{1/2}}[\exp(i\mathbf{K}_\perp\cdot\mathbf{R}_\perp)]\begin{pmatrix}\psi_{mn}(\mathbf{r},X)\\ \phi_{mn}(\mathbf{r},X)\\ \zeta_{mn}(\mathbf{r},X)\end{pmatrix}. \quad (3.13)$$

Since Φ_{mn} is the product of two functions of the form (2.13), we have

$$\phi_{mn}(\mathbf{r},X)=u_m(X+\tfrac{1}{2}x)u_n(X-\tfrac{1}{2}x)\exp(i\mathbf{k}_\perp\cdot\mathbf{r}_\perp), \quad (3.14)$$

where x is the x-component of $\mathbf{r}$. The partial wave amplitudes now depend on X as well as on r, and we write

$$\begin{pmatrix}\psi_{mn}(\mathbf{r},X)\\ \phi_{mn}(\mathbf{r},X)\\ \zeta_{mn}(\mathbf{r},X)\end{pmatrix}=\sum_{LM} i^M[4\pi(2L+1)]^{1/2}r^{-1}\begin{pmatrix}u_{LM}(r,X)\\ \phi_{LM}(r,X)\\ \zeta_{LM}(r,X)\end{pmatrix}Y_{LM}(\hat{r},\hat{x}), \quad (3.15)$$

where the factor i^M is inserted in order to make the radial functions real. By using (3.14) and (3.15), and taking $\mathbf{k}_\perp$ to point in the direction whose azimuth angle is zero, we obtain the formula

$$\phi_{LM}(r,X)=\left[\frac{(L-|M|)!}{(L+|M|)!}\right]^{1/2}\int_{-\frac{1}{2}r}^{\frac{1}{2}r} u_m(X+w)u_n(X-w)$$
$$\times J_M(k_\perp(r^2-4w^2)^{1/2})P_{LM}(2w/r)dw, \quad (3.16)$$

where J_M is a Bessel function, and P_{LM} is an associated Legendre polynomial.

The G matrix is easily found to be

$$\langle mn|G|mn\rangle=(4/\mathcal{A}N_mN_n)\int g_{mn}(X)dX, \quad (3.17)$$

where

$$g_{mn}(X)=\int \phi_{mn}^*(\mathbf{r},X)v\psi_{mn}(\mathbf{r},X)d^3r=\sum_{LM}4\pi(2L+1)$$
$$\times\int_0^\infty \phi_{LM}(r,X)v(r)u_{LM}(r,X)dr. \quad (3.18)$$

In order to use (3.18) for a potential with a hard core, we must derive a formula analogous to Rajaraman's result for nuclear matter which is given by (3.11). This can be accomplished by manipulating the equations satisfied by $\phi_{LM}(r,X)$ and $u_{LM}(r,X)$, and we therefore turn to a derivation of these equations.

The reference equation for the nuclear slab is easily written down by starting from the formula $e^RZ_{mn}=v\Psi_{mn}$ and using Eqs. (2.2) and (3.2) to find the explicit form of e^R. After eliminating the dependence on $\mathbf{R}_\perp$ and introducing partial waves, one finds

$$\left[\frac{\partial^2}{\partial r^2}-\frac{L(L+1)}{r^2}-\gamma_0^2+\frac{1}{4}\frac{\partial^2}{\partial X^2}\right]\zeta_{LM}(r,X)$$
$$=-m^*vu_{LM}(r,X), \quad (3.19)$$

where

$$\gamma_0^2=-m^*H+K_\perp^2/4. \quad (3.20)$$

Since $\phi_n(\mathbf{r})$ satisfies a simple one-body Schrödinger equation, and $\Phi_{mn}(\mathbf{r}_1,\mathbf{r}_2)$ is just the product of $\phi_m(\mathbf{r}_1)$ and $\phi_n(\mathbf{r}_2)$, it is easy to find the differential equation obeyed by Φ_{mn}. Then, after eliminating $\mathbf{R}_\perp$ and going to partial waves, one finds without difficulty that $\phi_{LM}(r,X)$ satisfies

$$\left[\frac{\partial^2}{\partial r^2}-\frac{L(L+1)}{r^2}+\tfrac{1}{2}(k_{mx}^2+k_{nx}^2)+\frac{1}{4}\frac{\partial^2}{\partial X^2}\right]\phi_{LM}(r,X)$$
$$=I_{LM}(r,X), \quad (3.21)$$

where

$$I_{LM}(r,X)=2U_0\int_{-\frac{1}{2}r}^{\frac{1}{2}r} u_m(X+w)u_n(X-w)F(w,X)\times J_M(k_\perp(r^2-4w^2)^{1/2})P_{LM}(2w/r)dw, \quad (3.22)$$

and

$$F(w,X)=(1+\exp[(X+w)/a])^{-1}+(1+\exp[(X-w)/a])^{-1}. \quad (3.23)$$

We can now obtain a useful expression for the radial integral of (3.18). By multiplying (3.19) by $\phi_{LM}(r,X)$ and (3.21) by $\zeta_{LM}(r,X)$, subtracting, and integrating from $r=0$ to $r=c^+$, we find a usable formula for the integral over the region of the hard core, and the final result is

$$\int_0^\infty \phi_{LM}(r,X)vu_{LM}(r,X)dr = \frac{\gamma_0^2+\frac{1}{2}(k_{mx}^2+k_{nx}^2)}{m^*}\int_0^c(\phi_{LM})^2dr + m^{*-1}\int_0^c \phi_{LM}I_{LM}dr+m^{*-1}\phi_{LM}(c)u_{LM}'(c+) + \int_{c+}^\infty \phi_{LM}vu_{LM}dr, \quad (3.24)$$

where the prime on u_{LM} indicates differentiation with respect to r. In deriving this equation, we have made use of the relation $u_{LM}=\phi_{LM}-\zeta_{LM}$ and the fact that $\phi_{LM}=\zeta_{LM}$ whenever $r\leq c$ and $\phi_{LM}\to 0$ as $r\to 0$.

The above formulas allow us to calculate the G matrix, either in infinite nuclear matter or in the nuclear slab, once the reference equation for u_{LM} has been solved in the region $r>c$. We consider S waves only and find from (2.10) that, in the case of nuclear matter, $\zeta_0(r)$ satisfies

$$\frac{d^2\zeta_0}{dr^2}-\gamma^2\zeta_0=-m^*v(\phi_0-\zeta_0), \quad (3.25)$$

and this equation can easily be solved numerically.

The reference equation in the surface region is given by (3.19) and can only be solved approximately because it contains derivatives with respect to both r and X. For values of X such that $|u_m(X)u_n(X)|$ is reasonably large, we can derive a useful approximation procedure by defining

$$\chi(r,x)=\zeta_0(r,X)/u_mu_n. \quad (3.26)$$

(The argument of u_m or u_n is understood to be X unless otherwise indicated.) The idea is that most of the X dependence of $\zeta_0(r,X)$ will be contained in the factor u_mu_n so that χ will depend weakly on X. Putting (3.26) into (3.19) gives, for S waves,

$$\left[\frac{\partial^2}{\partial r^2}-\gamma^2(X)\right]\chi(r,X)=-m^*v\left[\frac{\phi_0}{u_mu_n}-\chi\right] -\frac{1}{2u_mu_n}\frac{\partial\chi}{\partial X}\frac{d}{dX}(u_mu_n)-\frac{1}{4}\frac{\partial^2\chi}{\partial X^2}, \quad (3.27)$$

where we have defined

$$\gamma^2(X)=\gamma_0^2-\frac{1}{4u_mu_n}\frac{d^2}{dX^2}(u_mu_n). \quad (3.28)$$

In first approximation, the last two terms on the right-hand side of (3.27) are neglected. The resulting equation contains X only as a parameter and can be easily solved. In fact, it is of the same form as the nuclear-matter reference equation. By using the first approximation to estimate the neglected terms, one can obtain a second approximation, and this procedure can be continued indefinitely. It is found that the lowest order of this "χ approximation" gives sufficient accuracy in our case.

When X is near a zero of u_m or u_n, the χ approximation can no longer be used. Of course, this situation occurs in the outer part of the surface, where all single-particle wave functions decay to zero, but this very fact causes $g_{mn}(X)$ to be small in this region, and high accuracy is therefore not required. As we move through the surface towards the interior of the nucleus, however, we eventually reach the first node of u_m or u_n (see Fig. 2), and $g_{mn}(X)$ is not necessarily small here. The first node always occurs at a point which is sufficiently far inside the nucleus to allow u_m and u_n to be approximated by sine waves, and this fact permits us to solve (3.19) by a different approximation method.

Let us suppose, then, that for values of $|x|$ less than the range of the nuclear force, we can write

$$u_m(X+\tfrac{1}{2}x)\approx A_m\sin[p_m(X+\tfrac{1}{2}x)+\omega_m], \quad (3.29)$$

where A_m, p_m, ω_m are constants, with a similar expression for $u_n(X-\frac{1}{2}x)$. Then it is easy to show that the S-wave component of $\phi_{mn}(\mathfrak{r},X)$ is

$$\phi_0(r,X)\approx-\tfrac{1}{2}A_mA_n\cos[P_1X+\delta_1](\sin k_1r/k_1)+\tfrac{1}{2}A_mA_n\cos[P_2X+\delta_2](\sin k_2r/k_2), \quad (3.30)$$

where

$$P_1=p_m+p_n, \qquad P_2=p_m-p_n, \quad (3.31)$$

$$\delta_1=\omega_m+\omega_n, \qquad \delta_2=\omega_m-\omega_n, \quad (3.32)$$

$$k_1^2=k_1^2+\tfrac{1}{4}(p_m-p_n)^2, \quad k_2^2=k_1^2+\tfrac{1}{4}(p_m+p_n)^2. \quad (3.33)$$

If we now write

$$\zeta_0(r,X)=-\tfrac{1}{2}A_mA_n\cos[P_1X+\delta_1]\zeta_0^{(1)}(r)+\tfrac{1}{2}A_mA_n\cos[P_2X+\delta_2]\zeta_0^{(2)}(r), \quad (3.34)$$

and substitute (3.30) and (3.34) into the reference wave equation, we find that this equation splits into two

nuclear-matter equations, one for $\zeta_0^{(1)}$ and one for $\zeta_0^{(2)}$. Solving the reference equation in the surface region thus reduces to solving two nuclear-matter equations, adding the solutions, and weighting these solutions according to (3.34).

Thus we are able to calculate diagonal matrix elements of G, and exchange matrix elements are easily included by inserting in expression (3.18) a factor 3/4 for even values of L, and a factor 5/4 for odd L.

D. Surface Energy Formula

The nuclear slab can be specified by any three of the variables $\mathcal{A}$, L, A, k_F, where the Fermi momentum k_F is the momentum of the highest occupied single-particle state and A is the total number of nucleons. The details of the surface region, e.g. the behavior of the particle density and single-particle potential are, in principle, to be found from the self-consistency requirements. Note that the Fermi momentum k_F, which determines the interior particle density, is explicitly put into the calculation at the beginning. One should carry out a self-consistent calculation for each value of k_F; then the true nuclear ground state corresponds to the value of k_F which minimizes the total energy (for a fixed value of A). This is analogous to the procedure which one follows when calculating the properties of infinite nuclear matter.

Choosing A, $\mathcal{A}$, and k_F as independent variables, we can write for the total energy E of the nuclear slab,

$$E=Ag(k_F)+2\mathcal{A}S(k_F)+\cdots, \tag{3.35}$$

where terms of order $\mathcal{A}^{1/2}L$ and smaller, which are irrelevant for this discussion, have been omitted. We see that $g(k_F)$ is the energy per particle of nuclear matter with Fermi momentum k_F, and $S(k_F)$ is, by definition, the corresponding surface energy and is given by

$$S(k_F)=(E-Ag(k_F))/2\mathcal{A}. \tag{3.36}$$

Thus, $S(k_F)$ is found by calculating the total energy E, subtracting the energy the same number of particles would have if they were all located in infinite nuclear matter, and dividing the result by the total surface area.

The ground state value of k_F is the one which minimizes expression (3.35) for fixed $\mathcal{A}$, A. It is clearly equal, except for terms which vanish in the limit of a large system, to the equilibrium value for infinite nuclear matter, which we take to be 1.5 F^{-1}.

We want to write (3.36) in a more explicit form which is useful for calculations, but in order to do this we must first derive some preliminary results. We will need a summation formula, an identity involving the normalization of the wave functions, and an asymptotic formula for $g_{mn}(X)$ which is valid when the point X is in the interior of the nucleus.

We will calculate all quantities to first order in the Brueckner-Goldstone expansion, and this will involve summations over the occupied states ϕ_n, which we may label by the vector $\mathbf{k}_n\equiv(k_{nx},\mathbf{k}_\perp)$. We must, of course, approximate all such sums by integrals, and the approximation must be sufficiently accurate to cause the resulting error in the surface energy S to vanish as $\mathcal{A}$ and L tend to infinity.

For summing over $\mathbf{k}_\perp$, we will use the usual replacement

$$\sum_{\mathbf{k}_\perp}\rightarrow 4\frac{\mathcal{A}}{(2\pi)^2}\int d\mathbf{k}_\perp, \tag{3.37}$$

where the factor 4 takes account of spin-isospin degeneracy. When a function of order unity[20] is summed over $\mathbf{k}_\perp$ in this way, in order to evaluate E or A, the leading term is proportional to $\mathcal{A}$, and the error is of order $\mathcal{A}^{1/2}$. To evaluate expression (3.36), we must divide by $2\mathcal{A}$ and perform the sum over allowed values of k_x, i.e., we must sum a term of order unity, with an error of order $\mathcal{A}^{-1/2}$, over k_x. The sum of the error term over k_x gives a result of order $L\mathcal{A}^{-1/2}$, which vanishes in the limit $\mathcal{A}$, $L\rightarrow\infty$; hence, the replacement (3.37) is sufficiently accurate. Summing the accurate term of order unity over k_x gives a leading term of order L, a "first-order" term of order unity, and additional terms proportional to L^{-1} and smaller. We must find a formula for summing over k_x which gives both the leading term and the term of order unity correctly.

The sum over k_x of any function $f(k_x)$ can be considered as the sum over the integer n which labels allowed values of k_x according to (3.7). If f is a smooth function, it is then easy to show that the approximation

$$\sum_{n=1}^{nF} f(n)\rightarrow\int_{1/2}^{nF+\frac{1}{2}} f(n)dn \tag{3.38}$$

is in error by a quantity of order $L^{-1}(df/dk_x)_{\text{av}}$. So, if f and df/dk_x are both of order unity, the replacement (3.38) is sufficiently accurate for our purposes. Changing variables from n to k_x via (3.7), and noting that $n_F=k_FL/\pi-2\alpha(k_F)/\pi$, we easily deduce the formula

$$\sum_{k_x} f(k_x)=(L/\pi)\int_0^{kF} f(k_x)dk_x-(2/\pi)\int_0^{kF} f(k_x)\alpha'(k_x)dk_x+\tfrac{1}{2}[f(k_F)-f(0)], \tag{3.39}$$

which is accurate except for terms which vanish as $L\rightarrow\infty$ and is therefore acceptable for our computations.

In the interior of the nucleus, the one-particle wave functions are essentially sine waves, and this fact allows us to calculate the asymptotic form of $g_{mn}(X)$, which we call $\tilde{g}_{mn}(X)$, in terms of nuclear matter matrix elements. Neglecting exponentially small terms, we see

[20] We use the phrase "of order unity" to describe any quantity which remains finite as $A,L,\mathcal{A}$ tend to infinity.

from (3.6) and (3.14) that, when X is in the interior,

$$\phi_{mn}(\mathbf{r},X)=\exp(i\mathbf{k}_\perp\cdot\mathbf{r}_\perp)\sin[k_{nx}(X+\tfrac{1}{2}x)+\alpha_m]\times\sin[k_{nx}(X-\tfrac{1}{2}x)+\alpha_n]. \quad (3.40)$$

Clearly, $\phi_{mn}(\mathbf{r},X)$ can be written as a sum of nuclear matter wave functions (i.e., plane waves) and writing ϕ_{mn} in such a way induces a similar breakup of $\psi_{mn}(\mathbf{r},X)$ and $\zeta_{mn}(\mathbf{r},X)$ into nuclear matter functions (see the discussion of the sine wave approximation near the end of Sec. C).

The matrix element (3.18) for $g_{mn}(X)$ then becomes the following sum of nuclear matter matrix elements:

$$g_{mn}(X)=\tfrac{1}{8}\{g_{11}+g_{22}+\bar{g}_{11}\cos[2(k_{mx}+k_{nx})X+2(\alpha_m+\alpha_n)]+\bar{g}_{22}\cos[2(k_{mx}-k_{nx})X+2(\alpha_m-\alpha_n)]-(g_{12}+g_{21})\cos[2k_{nx}X+2\alpha_n]-(\bar{g}_{12}+\bar{g}_{21})\cos[2k_{mx}X+2\alpha_m]\}. \quad (3.41)$$

Here, we have made the definitions

$$\begin{pmatrix}g_{\beta\delta}\\ \bar{g}_{\beta\delta}\end{pmatrix}=\sum_{LM}4\pi(2L+1)\begin{pmatrix}1\\ (-1)^{L+M}\end{pmatrix}\int_0^\infty \phi_{LM}{}^{(\beta)}v u_{LM}{}^{(\delta)}dr, \quad (3.42)$$

where $\phi_{LM}{}^{(\beta)}$ and $u_{LM}{}^{(\delta)}$ are nuclear matter wave functions calculated for relative momentum k and total momentum K given by

$$k=[k_\perp{}^2+\tfrac{1}{4}(k_{mx}\mp k_{nx})^2]^{1/2} \quad (3.43)$$

$$K=[K_\perp{}^2+(k_{mx}\pm k_{nx})^2]^{1/2}. \quad (3.44)$$

(In these equations, the upper sign corresponds to superscript 1 and the lower sign to superscript 2.) In deriving a formula for the surface energy, we will also make use of the indefinite integral of $\tilde{g}_{mn}(X)$, which we call $\tilde{g}_{mn}{}^I(X)$ and which is given by

$$\tilde{g}_{mn}{}^I(X)=\tfrac{1}{8}\{(g_{11}+g_{22})X+\tfrac{1}{2}\bar{g}_{11}\sin[2(k_{mx}+k_{nx})X+2(\alpha_m+\alpha_n)]/(k_{mx}+k_{nx})+\tfrac{1}{2}\bar{g}_{22}\sin[2(k_{mx}-k_{nx})X+2(\alpha_m-\alpha_n)]/(k_{mx}-k_{nx})-\tfrac{1}{2}(g_{12}+g_{21})\sin[2k_{nx}X+2\alpha_n]/k_{nx}-\tfrac{1}{2}(\bar{g}_{12}+\bar{g}_{21})\sin[2k_{mx}X+2\alpha_m]/k_{mx}\}. \quad (3.45)$$

Next we define the quantity $\delta N(k_x)$ by

$$N_n=L+\delta N(k_{nx}), \quad (3.46)$$

and we derive the interesting and useful identity,

$$\delta N(k_x)=-2(d\alpha/dk_x). \quad (3.47)$$

This identity can be made plausible on physical grounds by noting that the spacing Δk_x between allowed values of k_x is given by

$$\Delta k_x=\pi/[L-2(d\alpha/dk_x)], \quad (3.48)$$

according to (3.7). But this is the spacing appropriate to a box of side $L-2(d\alpha/dk_x)$, and since particles of momentum k_x can be thought of as moving in a box whose "effective size" is $L+\delta N(k_x)$, it is quite natular to make the identification (3.47).

To demonstrate the truth of (3.47) mathematically, write the Schrödinger equation (3.4) for each of two wave functions $u_1(x)$ and $u_2(x)$, corresponding to momenta k_{1x} and k_{2x}, respectively. Multiply the equation for u_2 by u_1 and vice versa, subtract, and integrate from $-\frac{1}{2}L$ to ∞. After dividing the result by $(k_{2x}-k_{1x})$ and taking the limit $k_{2x}\to k_{1x}$, one obtains

$$\int_{-\frac{1}{2}L}^\infty |u_n(x)|^2dx=\frac{L}{4}-\frac{\sin(k_{nx}L-2\alpha)}{4k_{nx}}-\frac{1}{2}\frac{d\alpha}{dk_{nx}}. \quad (3.49)$$

For allowed values of k_x, the sine vanishes, and $|u_n(x)|^2$ is symmetric about $-\frac{1}{2}L$. Thus, we can write

$$2\int_{-\frac{1}{2}L}^\infty |u_n(x)|^2dx=\tfrac{1}{2}(L+\delta N)=\frac{L}{2}-\frac{d\alpha}{dk_x}, \quad (3.50)$$

from which (3.47) follows immediately.

We are now ready to derive a formula for the surface energy, and we consider first the kinetic energy contribution, which is denoted by $S(\text{K.E.})$. Since the kinetic energy per particle of infinite nuclear matter is $3k_F{}^2/10$, we see from (3.36) that

$$S(\text{K.E.})=\frac{1}{2\mathfrak{A}}\sum_n\langle n|T|n\rangle-\frac{1}{2\mathfrak{A}}\frac{3}{10}k_F{}^2\sum_1. \quad (3.51)$$

Let us consider first the evaluation of $(1/2\mathfrak{A})\sum_n 1$, which we may obviously write in the form

$$\frac{1}{2\mathfrak{A}}\sum_1=\frac{1}{2\mathfrak{A}}\sum_n\int|\phi_n(\mathbf{r})|^2d^3r. \quad (3.52)$$

Now, one can evaluate this expression by either of two distinct methods: One can first carry out the space integration for each n and then sum over n, or one can first sum over n for each point $\mathbf{r}$ and then integrate the result over all space. The first of these methods will be called the "summation method," and the second, which in this example amounts to integrating the particle density over all space, will be called the "density method."

Applying the summation method, we easily find, with the help of (3.39),

$$\frac{1}{2\mathfrak{A}}\sum_n 1=\frac{Lk_F{}^3}{3\pi^2}-\frac{1}{\pi^2}\times\int_0^{k_F}(k_F{}^2-k_x{}^2)\alpha'(k_x)dk_x-\frac{k_F{}^2}{4\pi}, \quad (3.53)$$

where $\alpha'(k_x)$ means $d\alpha/dk_x$, and we have dropped, as we always will, terms which vanish in the limit $\mathfrak{A}\to\infty$, $L\to\infty$.

If we now try to apply the density method, we find ourselves in difficulty at once. The trouble is that, far inside the nucleus, the percentage change in $\phi_n(\mathbf{r})$ between successive allowed values of k_x is large, and formula (3.39) is therefore not reliable for the calculation of the particle density $\rho(x)$, which is defined by

$$\rho(x)=\sum_n|\phi_n(\mathbf{r})|^2. \tag{3.54}$$

Nevertheless, we proceed to derive an approximate formula for $\rho(x)$. We perform the summation by using only the leading term of (3.39), and we replace N_n by L in expression (2.13) for $\phi_n(\mathbf{r})$, thereby obtaining

$$\rho(x)=\frac{2}{\pi^2}\int_0^{k_F}(k_F^2-k_x^2)|u(k_x,x)|^2dk_x. \tag{3.55}$$

One might expect to find an error of order L^{-1} in the last expression; hence, integrating it over the entire nucleus in order to evaluate $(1/2\mathcal{A})\sum_n 1$ would give the wrong answer.

The fact is, though, that using (3.55) to calculate $(1/2\mathcal{A})\sum_n 1$ leads to the correct expression given in (3.53). This can be shown by combining equations (3.52), (3.54), and (3.55), and by using (3.49) for the integral with respect to x of $|u(k_x,x)|^2$, to find

$$\frac{1}{2\mathcal{A}}\sum_n 1=\frac{2}{\pi^2}\int_0^{k_F}(k_F^2-k_x^2)\times\left[\frac{L}{4}-\frac{\sin(k_xL-2\alpha)}{4k_x}-\tfrac{1}{2}\alpha'(k_x)\right]dk_x. \tag{3.56}$$

Since $\alpha(k_x)\to 0$ as $k_x\to 0$, we have, for large L,

$$\frac{\sin(k_xL-2\alpha)}{4k_x}\approx\frac{\pi}{4}\delta(k_x), \tag{3.57}$$

and putting this into (3.56) leads to an expression which agrees perfectly with the correct result (3.53).[21] So we have demonstrated that the density method can be used to calculate $(1/2\mathcal{A})\sum_n 1$, with $\rho(x)$ given by the very simple formula (3.55).

Next we evaluate the quantity $(1/2\mathcal{A})\sum_n\langle n|T|n\rangle$, which can be written in the form

$$\frac{1}{2\mathcal{A}}\sum_n\int\phi_n^*(-\tfrac{1}{2}\nabla^2)\phi_n d^3r=\frac{1}{2\mathcal{A}}\sum_n\int[\tfrac{1}{2}\mathbf{k}_n^2-U_0(1+e^{-x/a})^{-1}]|\phi_n|^2d^3r, \tag{3.58}$$

where we have made use of the Schrödinger equation satisfied by $\phi_n(\mathbf{r})$. A straightforward application of the summation method yields

$$\frac{1}{2\mathcal{A}}\sum_n\langle n|T|n\rangle=\frac{Lk_F^5}{10\pi^2}-\frac{1}{4\pi^2}\int_0^{k_F}(k_F^4-k_x^4)\alpha'(k_x)dk_x-\frac{k_F^4}{16\pi}-\frac{2U_0}{\pi^2}\int_0^{k_F}(k_F^2-k_x^2)\times\int_{-\frac{1}{2}L}^{\infty}|u(k_x,x)|^2(1+e^{-x/a})^{-1}dxdk_x. \tag{3.59}$$

The computation of this quantity by means of the density method requires the evaluation of the kinetic energy density $\tau(x)$, which is given by

$$\tau(x)=\sum_n|\phi_n(\mathbf{r})|^2[\tfrac{1}{2}\mathbf{k}_n^2-U_0(1+e^{-x/a})^{-1}]. \tag{3.60}$$

Treating this formula in the same way as we treated (3.54), we obtain the approximate result

$$\tau(x)=\frac{1}{2\pi^2}\int_0^{k_F}(k_F^4-k_x^4)|u(k_x,x)|^2dk_x-U_0\rho(x)(1+e^{-x/a})^{-1}. \tag{3.61}$$

That this approximation is sufficiently accurate for the evaluation of $(1/2\mathcal{A})\sum_n\langle n|T|n\rangle$ is shown directly. Substituting (3.61) into the equation

$$\frac{1}{2\mathcal{A}}\sum_n\langle n|T|n\rangle=\int_{-\frac{1}{2}L}^{\infty}\tau(x)dx, \tag{3.62}$$

and carrying out the x integration before the $\mathbf{k}$ integration by means of (3.49), one easily obtains an expression which agrees with the correct result given in (3.59). Hence $(1/2\mathcal{A})\sum_n\langle n|T|n\rangle$ may be correctly evaluated by the density method, with formula (3.61) used for $\tau(x)$.

We can use our results to write two different but equivalent formulas for S(K.E.). The summation method gives, when (3.51), (3.53), and (3.59) are combined, the expression

$$S(\text{K.E.})=\frac{1}{\pi^2}\int_0^{k_F}(\tfrac{3}{5}k_F^2-k_x^2)k_x\alpha(k_x)dk_x+\frac{k_F^4}{80\pi}-\frac{2U_0}{\pi^2}\int_0^{k_F}(k_F^2-k_x^2)\times\left\{\int_{-\frac{1}{2}L}^{\infty}|u(k_x,x)|^2(1+e^{-x/a})^{-1}dx\right\}dk_x, \tag{3.63}$$

where we have integrated by parts and used the boundary condition $\alpha(k_x)\to 0$ as $k_x\to 0$. The density

[21] We must remember that only half of the δ-function peak contributes to the integral (3.56) because this integral runs only over positive values of k_x.

method, on the other hand, is easily seen to give

$$S(\text{K.E.})=\int_{-\frac{1}{2}L}^{\infty}[\tau(x)-\tfrac{3}{10}k_F{}^2\rho(x)]dx, \quad (3.64)$$

where $\rho(x)$ and $\tau(x)$ are given by (3.55) and (3.61), respectively.

Formula (3.63) is clearly suitable for numerical computation because the space integral in the last term receives appreciable contributions only from the surface region and can therefore be calculated numerically. But is the same thing true for the integral appearing in (3.64)? The answer is yes, and we show this by evaluating the contribution to the integral from values of X lying between $-\frac{1}{2}L$ and $-X_1$, where $-X_1$ is a point in the interior of the nucleus but far to the right of $-\frac{1}{2}L$ (i.e. X_1 is much larger than both $k_F{}^{-1}$ and the surface thickness, but $X_1\ll\frac{1}{2}L$). Using (3.55) and (3.61), we find

$$\int_{-\frac{1}{2}L}^{-X_1}[\tau(x)-\tfrac{3}{10}k_F{}^2\rho(x)]dx = \frac{1}{2\pi^2}\int_0^{k_F}(k_F{}^2-k_x{}^2)(k_x{}^2-\tfrac{1}{5}k_F{}^2)dk_x \times\int_{-\frac{1}{2}L}^{-X_1}|u(k_x,x)|^2dx, \quad (3.65)$$

where we have dropped a term involving $(1+e^{-x/a})^{-1}$, a quantity which is only appreciable in the surface region. Now, using the fact that $u(k_x,x)\sim-\sin(k_xx+\alpha)$ for $x\leq-X_1$, we find by a calculation similar to the derivation of (3.49), that

$$\int_{-\frac{1}{2}L}^{-X_1}|u(k_x,x)|^2dx = \frac{L-2X_1}{4}-\frac{\sin(k_xL-2\alpha)}{4k_x}+\frac{\sin(2k_xX_1-2\alpha)}{4k_x}. \quad (3.66)$$

But since L and $2X_1$ are both much larger than $k_F{}^{-1}$, each sine function in (3.66) equals $(\pi/4)\delta(k_x)$, and one cancels the other. The only surviving term in (3.66) is $(L-2X_1)/4$, and when this is substituted into (3.65), one easily finds that the right-hand side of (3.65) vanishes. Hence the contribution to the integral in (3.64) from any interval in x which is entirely outside the surface region is negligibly small. Thus, (3.64) is not only a correct formula but is also a useful one, because the integral can be evaluated accurately from a knowledge of the integrand for values of x in the surface region alone.

We now consider the potential energy contribution to the surface energy, which is denoted by $S(\text{P.E.})$ and is given to first order in the Brueckner-Goldstone expansion by

$$S(\text{P.E.})=\frac{1}{2\mathfrak{A}}\sum_{mn}\langle mn|G|mn\rangle-\frac{1}{2\mathfrak{A}}\bar{V}_N\sum_n 1. \quad (3.67)$$

In this expression, $\bar{V}_N$ represents the potential energy per particle of infinite nuclear matter and is given by either of the two equivalent expressions,

$$\bar{V}_N=(3/16\pi^4k_F{}^3)\int_{\text{whole sphere}}d^3k_md^3k_ng_{11} =(3\pi^2/k_F{}^2)(8\pi^6)^{-1} \times\int_{\text{half sphere}}d^3k_md^3k_n(g_{11}+g_{22}). \quad (3.68)$$

In the integral labeled "whole sphere," the variables are allowed to range over the entire Fermi sea, while "half sphere" means that both k_{mx} and k_{nx} are restricted to positive values.

Using (3.17), we can write the first term of (3.67) in the form

$$\frac{1}{2\mathfrak{A}}\sum_{mn}\langle mn|G|mn\rangle =\frac{2}{\mathfrak{A}^2}\sum_{mn}(1/N_mN_n)\int_{-\frac{1}{2}L}^{\infty}g_{mn}(X)dX. \quad (3.69)$$

To evaluate this by the summation method, we must calculate the integral for each pair of indices (m,n) and then sum over m and n. In the density method, we replace N_n, wherever it occurs, by L, and we use only the first term of (3.39) to sum over (m,n) inside the integral; then we integrate the resulting function of X between $-\frac{1}{2}L$ and ∞. We will first evaluate (3.69) rigorously, using the summation method, and then show that the same answer is obtained by the density method.

To apply the summation method, it is useful to write (3.69) in the form

$$\frac{1}{2\mathfrak{A}}\sum_{mn}\langle mn|G|mn\rangle =\frac{2}{\mathfrak{A}^2}\sum_{mn}\frac{1}{N_mN_n}\left\{\int_{-\frac{1}{2}L}^{X_0}(g_{mn}(X)-\tilde{g}_{mn}(X))dX +\int_{X_0}^{\infty}g_{mn}(X)dX+\tilde{g}_{mn}{}^I(X_0)-\tilde{g}_{mn}{}^I(-\tfrac{1}{2}L)\right\}, \quad (3.70)$$

where X_0 is an arbitrary point which we choose to lie in the surface region. For every term in the curly brackets except the last, we may replace N_n by L and use only the leading term of (3.39) for the summation, but the term involving $\tilde{g}_{mn}{}^I(-\frac{1}{2}L)$ requires more detailed examination. We find with the aid of (3.7) and (3.45) that

$$\tilde{g}_{mn}{}^I(-\tfrac{1}{2}L)=-(L/16)(g_{11}+g_{22}) +\tfrac{1}{8}\delta(k_{mx},k_{nx})\tilde{g}_{22}[-\tfrac{1}{2}L+\alpha'(k_{mx})], \quad (3.71)$$

where $\delta(k_{mx},k_{nx})$ is the Kronecker delta, and this result

may be substituted into (3.70) and the summation performed by means of (3.39). After using (3.47) and (3.68), and dropping terms which vanish in the limit of a large system, we finally obtain

$$\frac{1}{2\mathfrak{A}}\sum_{mn}{}^{\frac{1}{2}}\langle mn|G|mn\rangle=\frac{2}{\pi^6}\int_{\text{half sphere}}d^3k_m d^3k_n\left\{\int_{-\frac{1}{2}L}^{X_0}(g_{mn}-\tilde{g}_{mn})dX+\int_{X_0}^{\infty}g_{mn}dX+\tilde{g}_{mn}{}^I(X_0)\right\}+\frac{Lk_F{}^3}{3\pi^2}\bar{V}_N$$
$$-\frac{1}{8\pi^5}\int_{\substack{\text{half sphere,}\\ k_{nx}=0}}d^3k_m d^2k_{n\perp}(g_{11}+g_{22})+\frac{1}{8\pi^5}\int_{\substack{\text{half sphere,}\\ k_{nx}=k_{mx}}}d^3k_m d^2k_{n\perp}\bar{g}_{22}. \quad (3.72)$$

To evaluate (3.69) by the density method, we write

$$\frac{2}{\mathfrak{A}^2}\sum_{mn}\frac{1}{N_m N_n}\int_{-\frac{1}{2}L}^{\infty}g_{mn}(X)dX\rightarrow\int_{-\frac{1}{2}L}^{\infty}dX\frac{2}{\pi^6}\int_{\text{half sphere}}d^3k_m d^3k_n g_{mn}(X)$$
$$=\int_{-\frac{1}{2}L}^{X_0}dX\frac{2}{\pi^6}\int_{\text{half sphere}}d^3k_m d^3k_n(g_{mn}-\tilde{g}_{mn})+\int_{X_0}^{\infty}dX\frac{2}{\pi^6}\int_{\text{half sphere}}d^3k_m d^3k_n g_{mn}$$
$$+\frac{2}{\pi^6}\int_{\text{half sphere}}d^3k_m d^3k_n[\tilde{g}_{mn}{}^I(X_0)-\tilde{g}_{mn}{}^I(-\tfrac{1}{2}L)]. \quad (3.73)$$

In this last expression k_{mx} and k_{nx} are to be treated as continuous variables, and, since L is arbitrarily large, the sine functions in Eq. (3.45) for $g_{mn}(-\frac{1}{2}L)$ may be replaced by the appropriate Dirac delta functions. We substitute the resulting formula for $g_{mn}(-\frac{1}{2}L)$ into (3.73) and make use of the fact that when $k_{nx}=0$, we have $g_{12}=g_{21}=g_{11}=g_{22}$; and that if $k_{mx}=0$, it is true that $\bar{g}_{12}=\bar{g}_{21}=g_{11}=g_{22}$. There results a formula for $(1/2\mathfrak{A})^{\frac{1}{2}}\sum_{mn}\langle mn|G|mn\rangle$ which agrees perfectly with the correct expression (3.72). We therefore find that the density method is accurate, i.e., that the arrow in formula (3.73) may be replaced by an equality sign.

We can now collect our results and write two equivalent formulas for S(P.E.). Combining Eqs. (3.67), (3.72), and (3.53), we find

$$S(\text{P.E.})=\frac{2}{\pi^6}\int_{\text{half sphere}}d^3k_m d^3k_n\left\{\int_{-\frac{1}{2}L}^{X_0}(g_{mn}-\tilde{g}_{mn})dX+\int_{X_0}^{\infty}g_{mn}dX+\tilde{g}_{mn}{}^I(X_0)\right\}+\frac{1}{8\pi^5}\int_{\substack{\text{half sphere,}\\ k_{nx}=k_{mx}}}d^3k_m d^2k_{n\perp}\bar{g}_{22}$$
$$-\frac{1}{8\pi^5}\int_{\substack{\text{half sphere,}\\ k_{nx}=0}}d^3k_m d^2k_{n\perp}(g_{11}+g_{22})+\frac{2}{\pi^2}\bar{V}_N\int_0^{k_F}k_x\alpha(k_x)dk_x+\frac{k_F{}^2}{4\pi}\bar{V}_N. \quad (3.74)$$

The density method gives the much simpler formula

$$S(\text{P.E.})=\bar{V}_N\rho_0\int_{-\frac{1}{2}L}^{\infty}[W(X)-\rho(X)/\rho_0]dX, \quad (3.75)$$

where $\bar{V}_N$ and $\rho(X)$ are given by Eqs. (3.68) and (3.55), respectively, and $W(X)$ is defined by

$$W(X)=\frac{2}{\pi^2\bar{V}_N\rho_0}\int_{\text{half sphere}}d^3k_m d^3k_n g_{mn}(X). \quad (3.76)$$

Formula (3.74), though somewhat unwieldy, is clearly usable for computation because the space integrals receive appreciable contributions only from the surface region and hence can be correctly evaluated by numerical methods. The space integral in (3.75) also has this desirable property, as may be shown by a method similar to that previously used in the discussion of expression (3.64) for S(K.E.). Thus only the surface region contributes appreciably to the space integral in (3.75), and this formula is therefore useful for numerical computation.

The two formulas we have derived for the surface energy correspond to two complementary ways of looking at the physical origin of the surface energy. Consider the surface kinetic energy for example. Expression (3.63) for S(K.E.) was derived by a discrete summation over allowed states, while (3.64) is an energy density formula. The last term of (3.63) accounts for the loss of kinetic energy experienced by a particle which enters the surface region, where the one-particle potential becomes less attractive. The second term results from the fact that for a nucleus of finite size, the spectrum of allowed values of k_x does not extend all the way to zero as it does in

the case of infinite nuclear matter. The first term in (3.63) appears because the spacing between allowed values of k_x is not uniform, as it is for infinite nuclear matter, but decreases as k_x increases [this is because particles of higher momentum move in a larger region of configuration space; see the discussion of (3.47)].

Formula (3.64) for S(K.E.) gives rise to a completely different point of view and shows that we may, if we so desire, regard the surface energy as being localized in the surface region. This formula involves a comparison of the actual kinetic energy density $\tau(x)$ with the kinetic energy density which would prevail if $\tau(x)$ were proportional to $\rho(x)$. The two formulas for S(P.E.), although more complicated than those for S(K.E.), may be discussed and compared in the same way.

E. Numerical Results

In this section we give numerical results obtained by evaluating the various quantities occurring in the formulas for the surface energy. The calculations were performed on the Burroughs 220 and Control Data 1604 computers at the Cornell University Computing Center.

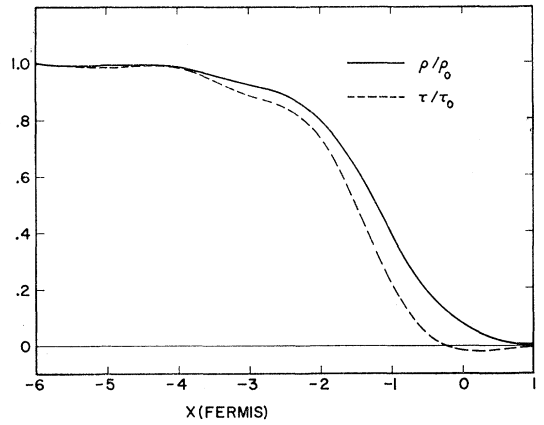

FIG. 1. Behavior of the particle density (solid curve) and kinetic energy density (dashed curve) in the surface region. Both quantities have been normalized by dividing by their asymptotic interior values, which are $\rho_0=2k_F^3/(3\pi^2)$ and $\tau_0=k_F^5/(5\pi^2)$.

Equation (3.4) was solved numerically in order to obtain the wave functions $u(x)$ and phase angles $\alpha(k_x)$ and then expressions (3.55) and (3.60) for $\rho(x)$ and $\tau(x)$ were evaluated. The resulting behavior of $\rho(x)$ and $\tau(x)$ in the surface region is shown in Fig. 1, and three of the one-particle wave functions are plotted in Fig. 2.

The particle density has a "90–10 distance" of 2.48F and falls to half its interior value at $x=-1.22$F. The kinetic energy density, of course, falls off more rapidly than the particle density (in the Thomas-Fermi approximation, for example, we have $\tau\propto\rho^{5/3}$). From the plot of the wave functions in Fig. 2, we see that particles with a high value of k_x penetrate the surface region extremely well, while particles of low momentum hardly "see" the surface at all.

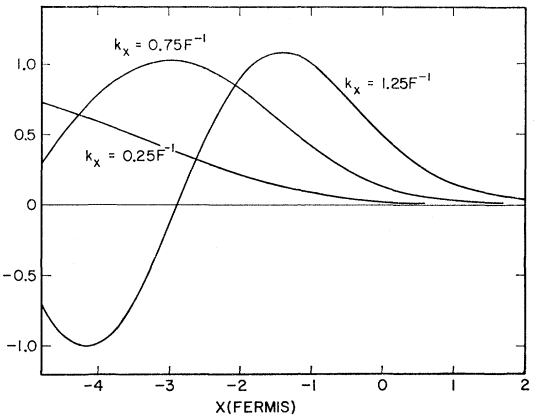

FIG. 2. Behavior of the one-particle wave function $u(x)$ in the surface region for three values of k_x.

The phase angle α is plotted as a function of k_x in Fig. 3. It is clear from the figure that $\delta N=-2d\alpha/dk_x$ is an increasing function of k_x, as we must expect.

By using the results just described, we evaluated the two equivalent expressions (3.63) and (3.64) for S(K.E.), obtaining a result of -2.48 MeV F^{-2} in each case. The values of the individual terms of (3.63) are shown in Table I, and we see that the loss of kinetic energy by a particle in the surface region is the dominant effect.

In order to evaluate the last four terms of Eq. (3.74) for S(P.E.), we must calculate diagonal nuclear matter matrix elements such as g_{11} and g_{22}. Such matrix elements depend only on the relative momentum k and total momentum K, and are easily obtained by numerically solving Eq. (3.25) and putting the result into (3.11). The dependence of the diagonal matrix element $g(k,K)$ on K is found to be very slight and almost quadratic. Its behavior as a function of k, for $K=0$, is shown in Fig. 4 and is similar to that obtained by Moszkowski and Scott[19] for the same two-body interaction but a different energy spectrum. The numerical results for the last four terms of (3.74) are given in Table I. The value obtained for $\bar{V}_N$ was -35.61 MeV, which gives a binding energy for infinite nuclear matter of 7.6 MeV particle.

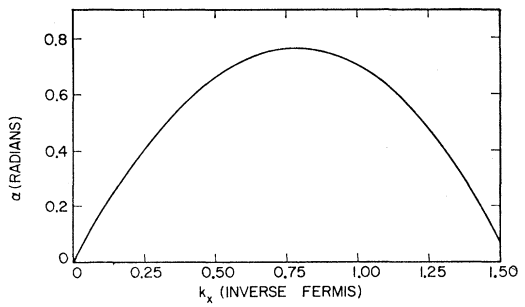

FIG. 3. The phase angle α as a function of k_x. In the interior of the nucleus, the one-particle wave function $u(x)$ has the form $-\sin(k_x x+\alpha)$.

In the first term of (3.74), the quantities $\tilde{g}_{mn}(X)$ and $\tilde{g}_{mn}{}^{I}(X)$ involve both diagonal and off-diagonal nuclear matter matrix elements, but these are easily obtained by solving (3.25) and using (3.11). The only part of the calculation which was at all time consuming for the Control Data 1604 computer was the evaluation of $g_{mn}(X)$. This required the computer first to calculate the functions $\phi_{LM}(r,X)$ and $I_{LM}(r,X)$ from formulas (3.16) and (3.22). Then Eq. (3.19) was solved for $u_{LM}(r,X)$ by one of the approximation methods previously discussed, and this result was used along with (3.24) and (3.18) to obtain $g_{mn}(X)$.

For a given pair (m,n) of interacting particles, $g_{mn}(X)$ was computed from $X=-5.20$ F up to $X=+1.0$ F in steps of 0.16 F, and this required 1.5 minutes of computer time. The χ approximation was used for X larger than -2.20 F, and the sine wave method was used for more negative values of X. It was estimated that the uncertainties in the surface energy caused by the use of the χ approximation and the sine wave approximation were 0.011 MeV F^{-2} and 0.014 MeV F^{-2}, respectively. So neither of these approximations affects the final result by more than 1%.

TABLE I. Values of the terms in the surface energy formula.

Terms in S(K.E.)	Value in MeV F^{-2}
$k_F{}^4/80\pi$	$+0.835$
$(1/\pi^2)\int_0^{k_F}(\frac{3}{5}k_F{}^2-k_x{}^2)k_x\alpha(k_x)dk_x$	$+1.003$
$-(2U_0/\pi^2)\int_0^{k_F}(k_F{}^2-k_x{}^2)dk_x$ $\times\int_{-\frac{1}{2}L}^{\infty}\lvert u_{kx}(x)\rvert^2(1+e^{-x/a})^{-1}dx$	-4.320
Total$=S$(K.E.)$=$	-2.482
Terms in S(P.E.)	
$(2/\pi^2)\bar{V}_N\int_0^{k_F}k_x\alpha(k_x)dk_x$	-4.353
$k_F{}^2\bar{V}_N$	-6.377
$(1/8\pi^5)\int_{\substack{\text{half sphere,}\\ k_{nx}=k_{mx}}}d^3k_m d^2k_{n\perp}\bar{g}_{22}$	-4.323
$-(1/8\pi^5)\int_{\substack{\text{half sphere,}\\ k_{nx}=0}}d^3k_m d^2k_{n\perp}(g_{11}+g_{22})$	$+13.676$
$(2/\pi^6)\int_{\text{half sphere}}d^3k_m d^3k_n$ $\times\{\int_{-\frac{1}{2}L}^{X_0}(g_{mn}-\tilde{g}_{mn})dX$ $+\int_{X_0}^{\infty}g_{mn}dX+\tilde{g}^I(X_0)\}$	$+5.286$
Total$=S$(P.E.)$=$	$+3.909$
$S=S$(K.E.)$+S$(P.E.)$=$	1.43

Some of the results for $g_{mn}(X)$ and $\tilde{g}_{mn}(X)$ are plotted in Fig. 5. The main feature is the large enhancement of the interaction of two particles in the surface region. As k_{nx} decreases from 1.375 F^{-1}, with k_{mx} fixed at 1.375 F^{-1}, the peak in $g_{mn}(X)$ becomes smaller because particles of low k_x do not penetrate the surface region very effectively. The very high final maximum in g_{mn} occurs because the wave functions u_m and u_n are especially large and because the momentum of each particle is reduced in the surface region. For $k_{mx}=k_{nx}=1.375$ F^{-1}, for example, $u_n(x)$ attains the value 1.11 at its last maximum in the surface region and since g_{mn} is roughly proportional to $\lvert u_m u_n\rvert^2$, this effect could increase g_{mn} by a factor of $(1.11)^4=1.52$. The reduction of momentum of each particle in the surface causes the relative momentum of two interacting particles to be smaller; so this effect also enhances the interaction in the surface region.

After the X integration involved in the first term of (3.74) had been carried out, the result was integrated over momentum space, and the final result is given in Table I. Adding up all the contributions gives a value of 3.91 MeV F^{-2} for S(P.E.) and a value of 1.43 MeV F^{-2} for the total surface energy S.

The largest computational uncertainty in this result arises from the coarseness of the mesh used in the k-space integration in the first term of (3.74). All other meshes were refined until the associated errors were negligible, but this procedure was not feasible for the first term of (3.74) because calculating the integrand at a single mesh point consumed 1.5 min on the computer. Since g_{mn} depends on the four variables k_{mx}, k_{nx}, $k_\perp$, $K_\perp$, and since the dependence on $K_\perp$ is quadratic and very weak, three of the six integrations involved in the phase-space

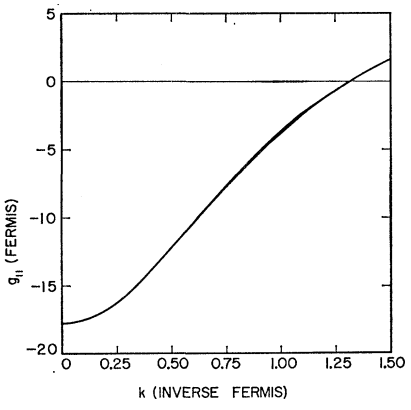

FIG. 4. The nuclear matter G-matrix element g_{11} as a function of the relative momentum k. The total momentum K of the interacting pair of particles is taken to be zero. To change the units of g_{11} from fermis to MeV F^3, one must multiply by 41.467.

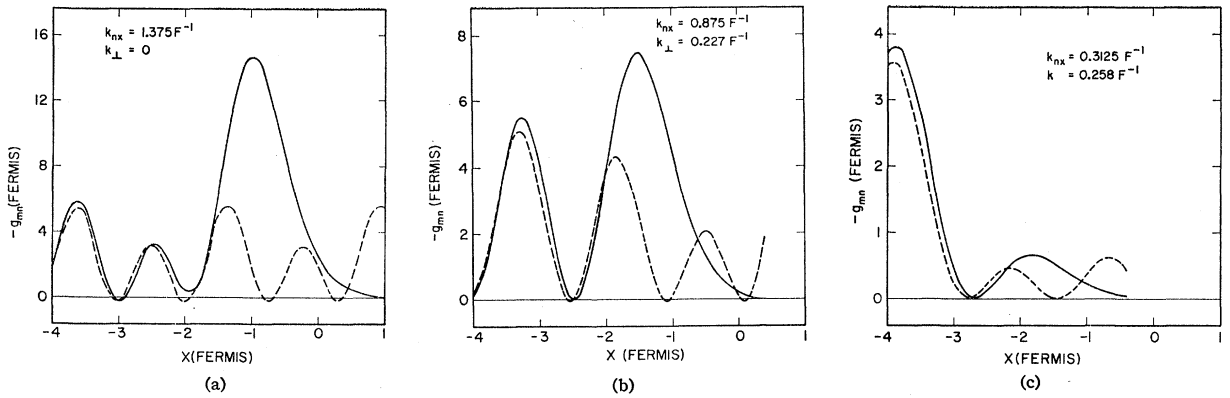

FIG. 5. The behavior of the effective two-body interaction $g_{mn}(X)$ in the surface region, for $k_{mx}=1.375$ F^{-1} and three different values of k_{nx}. The solid line represents $-g_{mn}(X)$, and the dashed line is a plot of $-\bar{g}_{mn}(X)$, the function to which $-g_{mn}(X)$ reduces in the interior of the nucleus. Note the different scales used on the vertical axes of the three graphs.

integral could be done analytically. The final three-dimensional integral with respect to k_{mx}, k_{nx}, $k_\perp$, was carried out by means of Simpson's rule, using a mesh with 88 points. The uncertainty produced in the surface energy by the use of this rather coarse mesh was estimated to be 0.07 MeV F^{-2}. The computational uncertainty from all sources in the final result of 1.43 MeV F^{-2} should be less than 0.10 MeV F^{-2}.

It is also of interest to calculate S(P.E.) by means of Eq. (3.75), but we are not able to evaluate this expression very accurately. The trouble is that $g_{mn}(X)$ varies rapidly with k_{mx} and k_{nx} when X is fairly large, and the k-space integral for $W(X)$ cannot be calculated accurately with the coarse mesh described above. We can estimate the range of X for which this mesh will give $W(X)$ correctly by noting that $g_{mn}(X)$ contains terms which vary like $\sin 2k_{mx}X$. If the spacing in k_{mx} or k_{nx} is Δk, then Simpson's rule should at best be accurate up to $|X|_{\max}$, where $2\Delta k|X|_{\max}=\pi/2$. Since Δk is about 0.25 on the average, we find $|X|_{\max}=\pi$. Thus, we may hope that numerical integration will give reasonable values of $W(X)$ for $X>-3$, but for $X<-3$, the values of $W(X)$ obtained in this way are probably useless.

The obvious solution to this difficulty is to use a finer mesh in the k space integration for $W(X)$. However, calculating the necessary values of $g_{mn}(X)$ would require many hours of additional computer time and was not felt to be worthwhile. Instead, we have used our 88-point mesh to calculate $W(X)$ for $X>-3$, and we have cut off the integral in (3.75) at this point. The result obtained for S(P.E.) in this way is 3.40 MeV F^{-2} which is 0.51 MeV F^{-2} below the correct value of 3.91 MeV F^{-2}. The functions $W(X)$ and $\rho(X)/\rho_0$ are plotted in Fig. 6, and it appears that there will be an appreciable contribution to the integral from the region $X<-3.0$ which will presumably account for the above discrepancy.

IV. CONCLUSION

We have seen that the reference spectrum for infinite nuclear matter can be generalized so as to apply to the surface of a large nuclear slab. When a simple reference spectrum approximation is used for the one-particle Hamiltonian of intermediate states, the G matrix in the surface region can be calculated to high accuracy by using the χ approximation and the sine wave approximation.

By using the "summation method" and the "density method," we have derived two distinct formulas for the surface energy which are valid to first order in the Brueckner-Goldstone expansion. These formulas are mathematically equivalent but are very different in appearance and represent two complementary ways of understanding the physical origin of the surface energy. In a given situation, one formula or the other may be more useful. For example, we were easily able to see from the energy density formula (3.64) that S(K.E.) must always be negative, but this fact is not obvious from expression (3.63) for S(K.E.), which is derived by the summation method. On the other hand, the summation method provides the more useful formula [Eq. (3.74)] for the numerical calculation of S(P.E.), at least in the case considered here. Although expression (3.74) is very unwieldy and consists of a large number of terms, most of which are considerably larger in magnitude than S(P.E.) itself, almost all of these terms involve only nuclear matter matrix elements and the

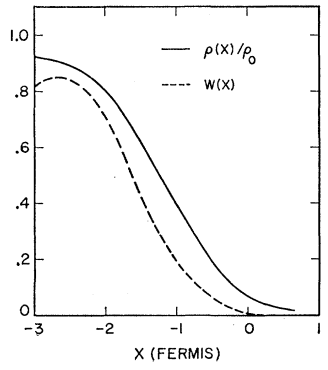

FIG. 6. The behavior of the functions $W(X)$ and $\rho(X)/\rho_0$ which appear in Eq. (3.75) for the surface potential energy.

phase angle $\alpha(k_x)$, and they can therefore be computed with great accuracy.

Our trial calculation gives a value for the surface energy of 1.43 MeV F^{-2}, and this corresponds to a term $20.6A^{2/3}$ MeV in the semiempirical mass formula for the total energy of a nucleus containing A nucleons. The semiempirical formulas of Green[22] and Cameron[23] give values of 17.97 MeV and 25.84 MeV, respectively, for this coefficient, and our result therefore seems to be reasonable.

The surface energy would be considerably larger if it were not for the large enhancement of the interaction between a pair of particles in the surface region, which is shown in Fig. 5. For instance, if $W(X)$ were proportional to $[\rho(X)/\rho_0]^2$, as is physically reasonable for a short-range two-body interaction, we would find $S(\text{P.E.})=4.59$ MeV F^{-2}, and the total surface energy would be 50% larger than it actually is.

The trial calculation gives a value of 7.6 MeV for the binding energy per particle of infinite nuclear matter, but the correct value is about 15 MeV. In order to correct this discrepancy, we might arbitrarily increase the strength of the two-body potential until $\bar{V}_N$ goes from -35.6 to -43.0 MeV, an increase in magnitude of 21%. Expression (3.75) would then increase by roughly the same percentage, and S(P.E.) would be increased from 3.91 to about 4.7 MeV F^{-2}. The calculated value for S would then increase from 1.43 to about 2.2 MeV F^{-2}, and this latter value corresponds to a coefficient in the semiempirical mass formula of 31.6 MeV, which is too large.

The most important shortcoming of the trial calculation presented here is the lack of self-consistency in the one-particle potential and wave functions. In addition to improving the calculation of the surface energy, a self-consistent determination of the wave functions of occupied states would lead to a theoretical prediction for the behavior of the particle density in the surface region. We have indicated how the methods of this paper could be used to investigate the self-consistency problem.

We have also used an oversimplified two-body interaction in our calculation. A realistic nucleon-nucleon potential has interaction in all partial waves, as well as tensor and spin-orbit forces. It may well be that the relative importance in the surface region of various partial waves, or of central, tensor, and spin-orbit forces, differs from that in infinite nuclear matter, and this could have an effect on the surface energy.

We have therefore made a beginning towards a detailed theory of the nuclear surface, but there remain a great many problems which require careful consideration. It is hoped that some of the results of this paper will be useful in this work.

ACKNOWLEDGMENTS

I want to express my sincere appreciation to Professor H. A. Bethe for suggesting this problem and for guiding me either through, or around, the various difficulties which arose in the course of the work. I also benefited greatly from discussions with B. Brandow and R. Rajaraman, and I want to thank Mrs. Joan Golowich and Miss Anne Walbran, of the Cornell University Computing Center, for helping me with the computer work. Financial assistance from the U. S. National Science Foundation and from Cornell University is gratefully acknowledged.

[22] A. E. S. Green, Phys. Rev. **95**, 1006 (1954).
[23] A. G. W. Cameron, Can. J. Phys. **35**, 1021 (1957).