Approximate Calculation of Nuclear Binding Energy*

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The binding energy, size, and shape of finite nuclei are studied using a method which tests the "local uniformity" assumption. This assumption implies that the properties of finite nuclei can be obtained from those of infinite nuclear matter. The energy is computed using as a trial wave function an amplitude- and frequency-modulated plane wave; this permits the use of nuclear-matter results in a straightforward manner. The calculation gives a binding energy which is too low, a radius which is too small, and a nuclear surface which is too diffuse. Several possible corrections to this result are examined.

I. INTRODUCTION

In recent years great progress has been made in understanding the gross properties of nuclei in terms of the two-body forces between nucleons. A natural starting point on this problem has been an investigation of the properties of uniform nuclear matter, that is, of an infinite medium of nucleons which can attain equilibrium if the Coulomb repulsion is neglected. The binding energy per particle and equilibrium density of nuclear matter have been successfully calculated by Brueckner and co-workers.[1] Saturation was obtained at a density which is only slightly higher than the central density found in electron-scattering experiments. In view of the approximations which are necessary to make the calculation manageable, and of the limitations inherent in any approach in which only the first term in a series is retained, the close correspondence with observation is quite remarkable. It does indeed suggest that the salient features of nuclear matter can be understood in terms of the two-body forces observed in scattering experiments, and that only two-body correlation effects are significant in the nuclear wave function.

One might now attempt to extend this approach to obtain a description of finite nuclei. A method which uses the infinite-medium results has been suggested by Brueckner, Gammel, and Weitzner.[2] This method is based on an approximation[3] which we shall call the "local uniformity assumption"; it is the purpose of this paper to investigate this assumption using a very simple model.[4]

The physical feature which underlies the local uniformity assumption is the observation that the range of nuclear forces is small compared to the observed falloff distance in finite nuclei. The all-important central even-state forces have ranges[5] in the triplet and singlet states of 0.5 f and 0.7 f, respectively; the longest-range force, the weak tensor odd-state force, has a range of 1.25 f.[6] The falloff distance of the nuclear density appears to be independent of mass number for heavy nuclei, with the 90-10 distance (the distance over which the density falls from 90% to 10% of its central value) approximately 2.5 f. The fact that the nuclear density varies slowly over the range of nuclear forces suggests that the properties of the nuclear medium within any small region of the nucleus should not be very different from those of an infinite medium of the same local density.

In the Brueckner approach[1] the nuclear forces and the pair correlations which they induce are described in terms of the K matrix. This is an integral solution of the Schrödinger equation for a pair of nucleons inside the nucleus, and hence depends upon the medium in which the two nucleons find themselves. For an infinite medium, the presence of the medium results in a density dependence of the K matrix. Brueckner, Gammel, and Weitzner[2] have obtained the spatial form of the K matrix for an infinite medium of arbitrary density. They find that the longer-range parts of the K matrix differ only slightly from the unmodified nuclear force, indicating that the relative wave function of the two nucleons is not greatly distorted by these parts of the force. The short-range part differs markedly from the force because of the hard core assumed in the nuclear force. This result shows that the correlation distance, i.e., the characteristic range of the distortion in the relative two-nucleon wave function, is very short. Consequently, it is found that only the contribution of the hard core, with its very short range, has a significant dependence on density. Because of this, it seems reasonable to assume that the K matrix is sensitive only to the local density.

It is basic to the Brueckner procedure that the nuclear medium be smooth and regular, since clustering is specifically neglected. In an infinite medium it has been

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[1] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958), hereafter called I, and references therein.
[2] K. A. Brueckner, J. L. Gammel, and H. Weitzner, Phys. Rev. **110**, 431 (1958), hereafter called II.
[3] This approximation has been used in a calculation of the spatial dependence of the imaginary potential. See G. L. Shaw, Ann. Phys. **8**, 509 (1959); L. C. Gomes, Phys. Rev. **116**, 1226 (1959).
[4] See L. Wilets, Revs. Modern Phys. **30**, 542 (1958), for a review of previous work on the nuclear surface.
[5] J. L. Gammel and R. M. Thaler, *Progress in Elementary Particle and Cosmic-Ray Physics* (North Holland Publishing Company, Amsterdam), Vol. V.
[6] We shall see in Sec. II that a more appropriate measure is the mean square radius, which is somewhat longer.

shown that many-particle correlation effects, or clusters, make negligible contributions to the binding energy. In extending the method to finite nuclei one would also assume, as a working hypothesis, that many-particle clusters are unimportant and that, as in the infinite medium, two-body correlations determine the many-body wave function.

We describe these hypotheses together as the "local uniformity assumption." We assume that (a) the K matrix, and hence the two-body correlations, at a point in the nucleus are determined only by the local density at that point, and (b) that cluster effects are not important.

II. METHOD

In the Brueckner approximation the total energy of an A-particle nucleus is

$$E=\langle\Phi_0|\sum_{i=1}^{A}T_i+\sum_{i<j}^{A}(K_{ij}+V_{cij})|\Phi_0\rangle \equiv\langle T\rangle+\langle K\rangle+\langle V_c\rangle, \quad (1)$$

where $T_i=-(\hbar^2/2m)\nabla_i^2$ is the kinetic energy operator, $K_{ij}=(\mathbf{r}_i\mathbf{r}_j|K|\mathbf{r}_i'\mathbf{r}_j')$ is the coordinate-space representation of the K matrix (the operator K is a matrix in the spin-charge space), $V_{cij}=(e^2/r_{ij})[(1+\tau_{zi})/2]\times[(1+\tau_{zj})/2]$ is the Coulomb potential, and Φ_0 is a determinant of single-particle wave functions: $\Phi_0=\det\Psi_i$. These functions can be determined by solving a modified Hartree-Fock equation[2,7] in which K_{ij} determines the single-particle potential. In principle K_{ij} depends upon Ψ_i, so that there is a complicated self-consistency problem if this dependence is retained. In the procedure proposed in II, the coordinate-space dependence of K_{ij} is obtained by Fourier-analyzing the momentum matrix elements of K. These in turn are obtained from a study[1] of infinite nuclear matter at the corresponding density. Thus K_{ij} is fixed, and the remaining equations involve the ordinary Hartree-Fock self-consistency condition, complicated by the fact that K_{ij} is a function of the local density.

We shall adopt a method which uses directly the results for infinite nuclear matter. However, rather than solve the very complicated integro-differential equations which determine Ψ_i, we shall replace Ψ_i by a simple trial function χ_i. In this way we can obtain analytic forms for the energy and examine explicitly the various surface terms that arise in finite nuclei. One can obtain[7] the modified Hartree-Fock equations for Ψ_i by minimizing Eq. (1) with respect to variations in Ψ_i. Thus we may expect that the energy which we obtain using our arbitrary function χ_i will be an upper limit to the energy which would be found by a correct Hartree-Fock procedure.

The spatial form that we shall choose for $\chi_i(r)$ is an amplitude- and frequency-modulated plane wave:

$$\chi_i(r)=f(r)e^{i\mathbf{k}_i(r)\cdot\mathbf{r}}\zeta_i\eta_i \quad (2)$$

(ζ_i and η_i are spin-charge functions). This is a natural generalization from the uniform plane waves of the infinite medium,[8] and should be a reasonable approximation for heavy nuclei. The amplitude modulation (which we choose to be real) represents the spatial density distribution in the nucleus; since the modulation factor $f(r)$ is independent of the state i, the density is simply

$$\rho(r)=Af^2(r), \quad (3)$$

provided $\int d^3r f^2(r)=1$. The frequency modulation (dependence of k_i on r) is intimately related to our use of the local uniformity assumption. Since we wish to treat the nucleus at every point as a nuclear medium having the local density, we must associate a Fermi momentum $k_F(r)$ with each point. Hence, the individual values of k_i, which are distributed uniformly between $k_i=0$ and $k_i=k_F$, must likewise depend upon the local density. The functions $\chi_i(r)$ do not form an orthogonal set, but one can show, using the methods of Drell and Huang,[9] that the lack of orthogonality causes a negligible error for large A.

To determine the dependence of k_i on r, we observe that

$$k_F(r)=[(3\pi^2/2)\rho(r)]^{\frac{1}{3}}. \quad (4)$$

This result includes the fact that each state $\chi_i(r)$ is occupied by four nucleons, and is obtained by replacing sums over states by integrals over momenta. The imposition of periodic boundary conditions leads to the form

$$\mathbf{k}_i(r)=(\mathbf{n}_i/n_F)k_F(r), \quad (5)$$

where n_i and n_F are integers. Hence, $k_i(r)$ has the same spatial dependence as $k_F(r)$, and is proportional to $\rho^{\frac{1}{3}}(r)$; the wave number decreases, and the wavelength increases, as r increases toward the less dense tail of the nuclear wave function.

We can now compute the expectation value of the kinetic energy using our trial function $\chi_i(r)$ and Eq. (3). There are three types of contributions, and we write

$$\langle T\rangle=T_0+(\delta T)_a+(\delta T)_f,$$

where

$$T_0=\int d^3r\left[\frac{3}{5}\frac{\hbar^2}{2m}k_F^2(r)\right]\rho(r),$$

$$(\delta T)_a=\frac{\hbar^2}{8m}\int d^3r\frac{1}{\rho}\left(\frac{d\rho}{dr}\right)^2, \quad (6)$$

$$(\delta T)_f=\int d^3r\left[\frac{3}{5}\frac{\hbar^2}{2m}k_F^2(r)\right]\left[\frac{4}{9}\frac{d\rho}{dr}\frac{r}{\rho}+\frac{1}{27}\frac{r^2}{\rho}\left(\frac{d\rho}{dr}\right)^2\right].$$

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

[8] Wave functions of this general form have been used previously. See for instance, P. Gombas, Acta Phys. Hung. **3**, 105 (1953); W. Wild and K. Wildermuth, Z. Naturforsch **9a**, 799 (1954).

[9] S. D. Drell and K. Huang, Phys. Rev. **91**, 1527 (1953), especially Appendix C.

T_0 is the average over the nuclear density of the kinetic energy of a Fermi gas. $(\delta T)_f$ is the correction to this arising from the frequency modulation which accompanies a change in the Fermi momentum. $(\delta T)_a$ is the correction arising from the amplitude modulation. This latter term has the form often used[4] in the statistical model. It has been shown by Berg and Wilets,[10] using some solvable examples, that it overestimates the surface energy; from our viewpoint this is a manifestation of the deviation of our trial function from the true wave function.

The nuclear force contribution to the potential energy is

$$\langle K\rangle=\sum_{i<j}\int dr_i dr_j dr_i' dr_j' \chi_i^*(r_i)\chi_j^*(r_j)(r_i r_j|K|r_i' r_j') \times[\chi_i(r_i')\chi_j(r_j')-\chi_j(r_i')\chi_i(r_j')]. \quad (7)$$

To facilitate discussion of the exchange term, we separate K into components which are diagonal in spin and isotopic spin:

$$K=\sum_{S,T} K_{ST}P_S{}^{\sigma}P_T{}^{\tau}, \quad (8)$$

where $P_S{}^{\sigma}$ and $P_T{}^{\tau}$ are projection operators on the spin and charge states, respectively. Thus

$$P_0{}^{\sigma}=\tfrac{1}{4}(1-\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j),$$
$$P_1{}^{\sigma}=\tfrac{1}{4}(3+\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j),$$

and similarly for $P_T{}^{\tau}$. The spatial representation of K_{ST} satisfies

$$(\mathbf{r}_i\mathbf{r}_j|K_{ST}|\mathbf{r}_i'\mathbf{r}_j')=-(-1)^{S+T}(\mathbf{r}_i\mathbf{r}_j|K_{ST}|\mathbf{r}_j'\mathbf{r}_i'), \quad (9)$$

since the two nucleons must have a symmetry under space exchange which is opposite to their symmetry under spin-charge exchange. If one now exchanges the variables of integration in the exchange term and uses the known symmetry properties of singlet-triplet states under exchange of coordinates, one finds that the exchange term is exactly equal to the direct term. This is, of course, a consequence of the built-in symmetry properties of the K matrix, as expressed in Eq. (9).

If we now assume that all spin-charge states are filled (closed shells), the sums over spin and charge can be easily performed. The result is

$$\langle K\rangle=2\sum_{i<j}\int dr_i dr_j dr_i' dr_j' f(r_i)f(r_j)e^{-i(\mathbf{k}_i\cdot\mathbf{r}_j+\mathbf{k}_j\cdot\mathbf{r}_j)} \times(\mathbf{r}_i\mathbf{r}_j|\bar{K}|\mathbf{r}_i'\mathbf{r}_j')\times e^{i(\mathbf{k}_i\cdot\mathbf{r}_i'+\mathbf{k}_j\cdot\mathbf{r}_j')}f(r_i')f(r_j'), \quad (10)$$

where

$$\bar{K}=\sum_{S,T}\frac{(2S+1)(2T+1)}{16}K_{ST}.$$

For the spatial dependence of the K matrix, we assume that

$$(\mathbf{r}_i\mathbf{r}_j|\bar{K}|\mathbf{r}_i'\mathbf{r}_j')=\delta(\mathbf{R}-\mathbf{R}')(\mathbf{r}|\bar{K}|\mathbf{r}'), \quad (11)$$

where

$$\mathbf{R}=(\mathbf{r}_i+\mathbf{r}_j)/2, \quad \mathbf{r}=\mathbf{r}_i-\mathbf{r}_j, \quad \text{etc.}$$

This is only an approximation since the δ function arises from Galilean invariance, i.e., invariance under velocity transformations. Translation invariance implies that $(\mathbf{r}_i\,\mathbf{r}_j|\bar{K}|\mathbf{r}_i'\,\mathbf{r}_j')$ can depend only on $\mathbf{R}-\mathbf{R}'$, $\mathbf{r}$, and $\mathbf{r}'$, but does not specify the functional dependence on these variables. In nuclear matter the K matrix is translation-invariant but is *not* Galilean-invariant, since the two particles are moving in a momentum-dependent potential. This causes $(\mathbf{k}_i\mathbf{k}_j|K|\mathbf{k}_i'\mathbf{k}_j')$ to depend on the total momentum $\mathbf{k}_i+\mathbf{k}_j=\mathbf{k}_i'+\mathbf{k}_j'$. The Fourier transform of $(\mathbf{k}_i\mathbf{k}_j|K|\mathbf{k}_i'\mathbf{k}_j')$ is thus not local in the center-of-mass coordinate. (One can, of course, see this in coordinate space also, where the single-particle potential is nonlocal.) However, it was found in I (and assumed in II) that the dependence on the total momentum is weak, so that Eq. (11) is expected to be a valid approximation.

By making use of our assumption that the range of the two-body force is small compared to the nuclear falloff distance, we shall expand the amplitude- and frequency-modulation functions about the two-particle center of mass. Keeping terms of order r^2,

$$f(r_i)=f(R)+\frac{\mathbf{r}\cdot\mathbf{R}}{2R}\frac{df(R)}{dR}+\frac{1}{8}\frac{r^2R^2+(\mathbf{r}\cdot\mathbf{R})^2}{R^3}\frac{df(R)}{dR} +\left(\frac{\mathbf{r}\cdot\mathbf{R}}{R}\right)^2\frac{d^2f(R)}{dR^2}. \quad (12)$$

In the product $f(r_i)f(r_j)$, the term of order r cancels out. After performing an average over the angles of $\mathbf{R}$ and using Eq. (3), we find

$$f(r_i)f(r_j)=A^{-1}\rho(R) \times\left\{1+\frac{r^2}{12}\left[\frac{1}{R}\frac{d\ln\rho(R)}{dR}+\frac{1}{2}\frac{d^2\ln\rho(R)}{dR^2}\right]\right\}+\cdots. \quad (13)$$

Similarly, if we expand $k_i(r_i)$ about the center of mass, we find, to order r^2,

$$e^{i\mathbf{k}_i(r_i)\cdot\mathbf{r}_i}=e^{i\mathbf{k}_i(R)\cdot\mathbf{r}_i}\left\{1+i\frac{\mathbf{k}_i\cdot\mathbf{r}_i}{k_i}\left[\frac{\mathbf{r}\cdot\mathbf{R}}{2R}\frac{dk_i(R)}{dR} +\frac{1}{8}\frac{r^2R^2-(\mathbf{r}\cdot\mathbf{R})^2}{R^3}\frac{dk_i(R)}{dR}+\frac{1}{8}\left(\frac{\mathbf{r}\cdot\mathbf{R}}{R}\right)^2\frac{d^2k_i(R)}{dR^2}\right] -\frac{1}{8}\left(\frac{\mathbf{k}_i\cdot\mathbf{r}_i}{k_i}\right)^2\left(\frac{\mathbf{r}\cdot\mathbf{R}}{R}\right)^2\left(\frac{dk_i(R)}{dR}\right)^2+\cdots\right\}. \quad (14)$$

If we take the product of the two plane waves, drop those terms which are linear in $\mathbf{R}$ and hence vanish upon

[10] R. A. Berg and L. Wilets, Proc. Phys. Soc. (London) **A68**, 229 (1955); R. A. Berg and L. Wilets, Phys. Rev. **101**, 201 (1956).

integration over $\mathbf{R}$, and use Eq. (4), we obtain

$$e^{i\mathbf{k}_i\cdot(\mathbf{r}_i)\cdot\mathbf{r}_i}e^{i\mathbf{k}_j\cdot(\mathbf{r}_j)\cdot\mathbf{r}_j}=e^{i\mathbf{K}\cdot\mathbf{R}}e^{i\mathbf{k}\cdot\mathbf{r}}\Big\{1+i\frac{(\mathbf{k}\cdot\mathbf{R})(\mathbf{r}\cdot\mathbf{R})}{3R}\frac{d\ln\rho(R)}{dR}$$
$$-\frac{1}{18}(\mathbf{k}\cdot\mathbf{R})^2\left(\frac{\mathbf{r}\cdot\mathbf{R}}{R}\right)^2$$
$$\times\left[\frac{d\ln\rho(R)}{dR}\right]^2+\cdots\Big\}. \quad (15)$$

We have suppressed the dependence of k and K on R, i.e., $k\equiv k(R)$, etc. Before inserting these into Eq. (10), it is convenient to examine the form of the leading term in these expansions. Using Eq. (11), the leading term is

$$V_0=2\sum_{i<j}\int d^3Rd^3rd^3r'\,A^{-2}\rho^2(R)e^{-i\mathbf{k}\cdot\mathbf{r}}$$
$$\times(\mathbf{r}|\bar{K}(\rho)|\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'}. \quad (16)$$

This can be simply expressed in terms of the nuclear-matter results of I in the following way. In a medium of uniform density the potential energy is

$$V(\rho)=2\sum_{i<j}(\mathbf{k}_i\mathbf{k}_j|\bar{K}(\rho)|\mathbf{k}_i\mathbf{k}_j), \quad (17)$$

where

$$(\mathbf{k}_i\mathbf{k}_j|\bar{K}(\rho)|\mathbf{k}_i\mathbf{k}_j)=\frac{1}{v}\int d^3rd^3r'\,e^{-i\mathbf{k}\cdot\mathbf{r}}(\mathbf{r}|\bar{K}(\rho)|\mathbf{r}')e^{i\mathbf{k}\cdot\mathbf{r}'}.$$

v is the "normalization volume" which is conventionally used to define the momenta $\mathbf{k}_i$. Thus v is related to the Fermi momentum by

$$\frac{v}{(2\pi)^3}\frac{4\pi}{3}k_F^3=\frac{A}{4}.$$

Comparing with Eq. (4), we see that

$$1/v=A^{-1}\rho.$$

Therefore,

$$V_0=\int d^3R\,A^{-1}\rho(R)V(\rho); \quad (18)$$

this is just the average over the nuclear density of the potential energy of a uniform medium. $V(\rho)$ is related to the energy per particle (excluding Coulomb energy) of a medium of density ρ by

$$E_b(\rho)=\frac{3}{5}\frac{\hbar^2k_F^2}{2m}+\frac{1}{A}V(\rho). \quad (19)$$

Hence, the leading terms in the energy can be combined to give

$$E_0=T_0+V_0=\int d^3R\,\rho(R)E_b(\rho). \quad (20)$$

This is just an average over the nuclear density of the energy of nuclear matter.

If we now insert Eqs. (13) and (15) into Eq. (10), we find

$$\langle K\rangle=V_0+(\delta V)_f+(\delta V)_a,$$

where V_0 is given by Eq. (18),

$$(\delta V)_f=\int d^3R\,A^{-1}\rho(R)V(\rho)\Big\{i\frac{R}{9}\langle(\mathbf{k}\cdot\mathbf{s})\rangle_{\rm av}\frac{d\ln\rho(R)}{dR}$$
$$-\frac{R^2}{135}[\langle(\mathbf{k}\cdot\mathbf{s})^2\rangle_{\rm av}+\tfrac{1}{2}\langle k^2s^2\rangle_{\rm av}]\left[\frac{d\ln(R)}{dR}\right]^2\Big\}, \quad (21)$$

with $\mathbf{s}=\mathbf{r}'-\mathbf{r}$, and

$$(\delta V)_a=\int d^3R\,A^{-1}\rho(R)V(\rho)\frac{\langle r^2\rangle_{\rm av}}{6}$$
$$\times\left[\frac{1}{R}\frac{d\ln\rho(R)}{dR}+\frac{1}{2}\frac{d^2\ln\rho(R)}{dR^2}\right].$$

We have performed the integrals over the angles of $\mathbf{R}$ in order to simplify the expressions. In $(\delta V)_a$ we have used the fact that $\langle\mathbf{r}|K(\rho)|\mathbf{r}'\rangle$ is Hermitian, so that $\langle r^2\rangle_{\rm av}=\langle r'^2\rangle_{\rm av}$.

The averages in Eq. (21) are functions of the density $\rho(R)$, and are defined by

$$\langle g(\mathbf{k};\mathbf{r},\mathbf{r}')\rangle_{\rm av}$$
$$=\frac{2A^{-1}\rho(R)\sum_{i<j}\int d^3rd^3r'\,e^{-i\mathbf{k}\cdot\mathbf{r}}\langle\mathbf{r}|\bar{K}(\rho)|\mathbf{r}'\rangle e^{i\mathbf{k}\cdot\mathbf{r}'}g(\mathbf{k};\mathbf{r},\mathbf{r}')}{V(\rho)}. \quad (22)$$

Thus $g(\mathbf{k},\mathbf{r},\mathbf{r}')$ is an average, weighted by the effective potential $\langle\mathbf{r}|\bar{K}(\rho)|\mathbf{r}'\rangle$, over coordinate space and over the filled states of the Fermi sea.

$(\delta V)_f$ is a correction arising from the nonlocality of the K matrix. If the K matrix were local, i.e., if $\langle\mathbf{r}|\bar{K}(\rho)|\mathbf{r}'\rangle=\bar{K}(\rho;r)\delta(\mathbf{s})$, $(\delta V)_f$ would vanish. This is a consequence of the fact that for a local K matrix there is no dependence on the momentum of the particles. Because of the nonlocality $(\mathbf{k}_i\mathbf{k}_j|\bar{K}(\rho)|\mathbf{k}_i\mathbf{k}_j)$ does depend upon $\mathbf{k}_i$ and $\mathbf{k}_j$. $(\delta V)_f$ is the energy correction which reflects the variation of these momenta over the range of the nonlocality. We shall see shortly that this correction is small compared to $(\delta V)_a$.

$(\delta V)_a$ is a correction due to the variation in nuclear density over the range of the nuclear force. This is analogous to the classical surface tension, which arises from a nonuniform distribution of particles. It is reasonable physically that $(\delta V)_a/V_0$ is of order $\langle(r/t)^2\rangle_{\rm av}$ where t is the nuclear falloff distance. (This will be seen in the specific example discussed below.) On the other hand, $(\delta V)_f/V_0$ is of order $(k_Fs_0)^2$, where s_0 is the range of the nonlocality. [This follows most simply from the observation, based on reflection invariance, that $(\delta V)_f$ must be an even function of k_F and of s_0.]

If we use the results of II, the "mean square radius"[11] of the effective potential is $\langle r^2\rangle_{\rm av}=3.5$ f^2 while the range of the nonlocality is less than 0.2 f. From electron scattering experiments[12] the nuclear falloff distance is approximately 2.5 f. Finally, $k_F\cong 1.3$ f^{-1} at the central density. Thus, $(k_F s_0)^2\lesssim 0.068$ while $\langle(r/t)^2\rangle_{\rm av}\cong 0.56$. Hence, we expect $(\delta V)_f/(\delta V)_a\sim 10\%$; in fact, it turns out to be considerably smaller than this.

III. CALCULATION

One could obtain the minimum energy consistent with the trial function Eq. (2) by setting $\delta\langle E\rangle/\delta\rho=0$. This would yield a differential equation for $\rho(R)$ which would require numerical solution.[4,10] We shall instead assume an analytic form for $\rho(r)$ which depends on two variational parameters.[13] These will determine the radius and falloff distance of the distribution.

A convenient form is the "generalized Gaussian"[14]

$$\rho(R)=\rho_0\exp[-(R/R_0)^n]. \tag{23}$$

This is a very general form which encompasses the observed Gaussian shape of light nuclei and the Fermi-type density of heavy nuclei having a large central region of constant density.

All the integrals which we need can be evaluated in terms of gamma functions provided only that $V(\rho)$ is represented by a polynomial in ρ (of arbitrary integral or nonintegral order). In fact, the general integral which we encounter is

$$I_q{}^m=\int d^3R\, R^q[\rho(R)]^m =4\pi\frac{\rho_0{}^m}{n}\left(\frac{R_0{}^n}{m}\right)^{(q+3)/n}\Gamma\left(\frac{q+3}{n}\right). \tag{24}$$

The normalization condition

$$\int d^3R\,\rho(R)=A, \tag{25}$$

implies that

$$\rho_0=\frac{A}{(4\pi/3)R_0{}^3\Gamma(1+3/n)}. \tag{26}$$

The radius at half-maximum density is

$$c=(\ln 2)^{1/n}R_0=R_0(1-0.368/n+\cdots), \tag{27}$$

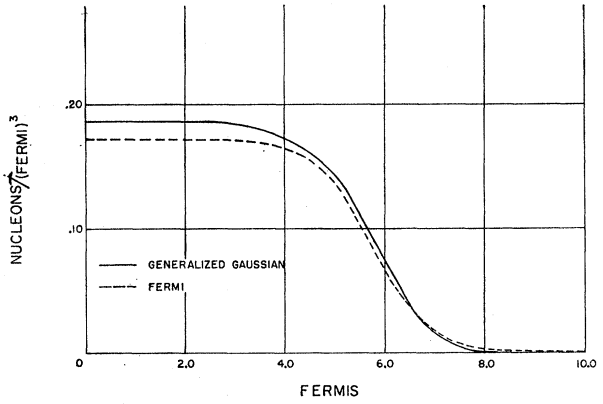

FIG. 1. Comparison of the generalized Gaussian function, Eq. (23), with the Fermi distribution $\rho'_0[1+e^{(r-c)/a}]^{-1}$, for $A=150$. The parameters are chosen to give the same half-density distance $c=5.73$ f and falloff distance $t=2.5$ f.

while the 90%-10% falloff distance is

$$t=\left[(\ln 10)^{1/n}-\left(\ln\frac{10}{9}\right)^{1/n}\right]R_0 =\frac{3.08R_0}{n}\left(1-\frac{0.715}{n}+\cdots\right). \tag{28}$$

Electron scattering experiments[12] indicate that, for $A>100$, these parameters are $c=r_1A^{\frac{1}{3}}$ with $r_1=1.08\pm 0.02$ f while $t=2.5\pm 0.3$ f, independent of A. These values imply the relations

$$\begin{aligned} R_0&\cong(1.08A^{\frac{1}{3}}+0.30)\text{ f},\\ n&\cong 1.33A^{\frac{1}{3}}-0.35, \end{aligned} \tag{29}$$

for large A. For heavy nuclei $n\sim 7$. In Fig. 1 the generalized Gaussian distribution is compared with a Fermi distribution having the same values of c and t, for $A=150$.

The Coulomb energy is

$$\langle V_c\rangle=\sum_{i<j}\int d^3r_i d^3r_j\, f^2(r_i)f^2(r_j) \times\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}\left(\frac{1+\tau_{3i}}{2}\right)\left(\frac{1+\tau_{3j}}{2}\right)-\text{exchange}. \tag{30}$$

The exchange term can be calculated,[15] but it is found to be quite small (of the order of several tenths of Mev) and shall not be included in our further considerations. Since

$$\sum_{i<j}\left(\frac{1+\tau_{3i}}{2}\right)\left(\frac{1+\tau_{3j}}{2}\right)=\frac{Z(Z-1)}{2}\cong\frac{Z^2}{2},$$

[11] It should be noted that this radius does not have the usual physical interpretation as a mean square interaction radius, since the K matrix is nonmonotonic. For a nonmonotonic function $\langle r^2\rangle_{\rm av}$ has no such simple interpretation, and can indeed be negative.

[12] R. Hofstadter, Revs. Modern Phys. 28, 214 (1956).

[13] The electron scattering experiments which have been performed[12] thus far can determine only two independent density parameters, such as the half-density radius and the falloff distance.

[14] The use of this function was suggested to one of us (L.S.R.) by Professor F. Villars in connection with an investigation of the nuclear symmetry energy.

[15] H. A. Bethe and R. F. Bacher, Revs. Modern Phys. 8, 82 (1936).

$$E_c=\langle V_c\rangle\cong\frac{1}{2}\left(\frac{Z}{A}\right)^2 e^2\int d^3r_1 d^3r_2\frac{\rho(r_1)\rho(r_2)}{|\mathbf{r}_1-\mathbf{r}_2|}$$
$$=\left(4\pi\frac{Z}{A}e\right)^2\int_0^\infty r_1 dr_1\,\rho(r_1)\int_0^{r_1} r_2^2 dr_2\,\rho(r_2). \quad (31)$$

This can be computed exactly, using Eq. (23), for $n=1$, 2, and 3. Letting $E_c=\frac{3}{5}(Ze)^2/R_{\text{eff}}$, the effective radius is

$$R_{\text{eff}}/R_0=96/25=3.84 \quad \text{for} \quad n=1$$
$$=\tfrac{3}{5}(2\pi)^{\frac{1}{2}}\cong 1.50 \quad \text{for} \quad n=2$$
$$=\tfrac{2}{5}\{[1-(\tfrac{1}{2})^{\frac{3}{2}}]\Gamma(5/3)\}^{-1}\cong 1.21 \quad \text{for} \quad n=3. \quad (32a)$$

For large n we may make use of the fact that the expectation value of the long-range Coulomb potential is insensitive to the shape of the density function $\rho(r)$. Thus, we perform an expansion of $\rho(r)$ in which the leading term is simply a uniform sphere. Using Eq. (23), this is just a Taylor expansion about $n=\infty$ or, more conveniently, about $1/n=0$:

$$\rho(r)=\rho_0\exp[-(r/R_0)^n]$$
$$=\rho_0\left[u(R_0-r)+\Gamma'(1)\frac{R_0}{n}\delta(r-R_0)+O\left(\frac{1}{n^2}\right)\right], \quad (33)$$

where

$$u(R_0-r)=1, \quad r<R_0$$
$$=0, \quad r>R_0$$

and $\delta(r-R_0)$ is the Dirac δ function. Also $\Gamma'(1)=[d\Gamma(z)/dz]_{z=1}=0.577$. Using this expansion and the expansion of $\Gamma(1+3/n)$, we find

$$R_{\text{eff}}=R_0\left[1+\frac{\Gamma'(1)}{n}+O\left(\frac{1}{n^2}\right)\right]$$
$$\cong R_0\left[\Gamma\left(1+\frac{3}{n}\right)\right]^{\frac{1}{3}} \quad \text{for} \quad n\to\infty. \quad (32b)$$

This is just the radius of the equivalent uniform sphere having the same volume as $\exp[-(r/R_0)^n]$.

We now want to examine the numerical consequences of this model. To facilitate numerical computation $E_b(\rho)$ (Fig. 1 of I) is fit with a polynomial in $\rho^{\frac{1}{3}}$:

$$E_b(\rho)=a_2\rho^{\frac{2}{3}}+a_3\rho+a_4\rho^{\frac{4}{3}}, \quad (34)$$

where

$$a_2=-19.5 \text{ Mev},$$
$$a_3=-188 \text{ Mev},$$
$$a_4=253 \text{ Mev}.$$

This provides an accurate fit over the region which was included in I (densities down to 0.3 of the equilibrium density) and vanishes for small ρ.

In calculating $(\delta V)_f$ and $(\delta V)_a$ we shall make the simplifying, but quite accurate, assumption that the various averages $\langle g(\mathbf{k};\mathbf{r},\mathbf{r}')\rangle_{\text{av}}$ are independent of density. We can determine $\langle r^2\rangle_{\text{av}}$ using the results of II, where it is shown that the long-range part of the K matrix, which is predominant in $\langle r^2\rangle_{\text{av}}$, is nearly independent of density. Using II [especially Figs. 3 and 4 and Eq. (54)] we find $\langle r^2\rangle_{\text{av}}=3.5$ f^2. To estimate the averages which occur in $(\delta V)_f$, we have represented the K matrix by a product

$$(\mathbf{r}|\bar{K}|\mathbf{r}')=[K(\mathbf{r})+K(\mathbf{r}')]\exp[-(s/s_0)^2], \quad (35)$$

where $\mathbf{s}=\mathbf{r}'-\mathbf{r}$. The results of II indicate that $s_0\cong 0.15$ f. We find $-i\langle\mathbf{k}\cdot\mathbf{s}\rangle_{\text{av}}=\langle\mathbf{k}\cdot\mathbf{s}\rangle^2_{\text{av}}=(3/20)(k_F s_0)^2$ and $\langle k^2 s^2\rangle_{\text{av}}=(9/20)(k_F s_0)^2$, dropping terms of order $(k_F s_0)^4$. These results are independent of the form of $K(\mathbf{r})$.

TABLE I. Individual contributions to the energy per particle. Column A: general form using Eq. (23). Column B: values obtained with the observed nuclear shape, Table II, Column A. Column C: values obtained by minimizing the energy; the corresponding shape parameters are given in Table II, Column B. The numerical values of the Coulomb energy in Columns B and C were obtained by interpolation using Eqs. (32a) and (32b). The coefficients a_i are given by Eq. (34). The coefficient a_2' is given by $a_2'=a_2-\frac{3}{5}(\hbar^2/2m)(3\pi^2/2)^{\frac{2}{3}}$. Energies are measured in Mev/particle.

A	B	C
$\frac{E_0}{A}=\left(\frac{3}{5}\right)^{3/n}a_2\rho_0^{2/3}+\left(\frac{1}{2}\right)^{3/n}a_3\rho_0+\left(\frac{3}{7}\right)^{3/n}a_4\rho_0^{4/3}$	−12.4	−10.7
$\frac{(\delta T)_a}{A}=\frac{\pi\hbar^2}{2m}\frac{nR_0}{A}\Gamma\left(2+\frac{1}{n}\right)\rho_0$	3.5	1.9
$\frac{(\delta T)_f}{A}=\frac{3}{5}\frac{\hbar^2}{2m}\frac{n-7}{25}\left(\frac{3}{5}\right)^{3/n}\left(\frac{3\pi^2}{2}\rho_0\right)^{2/3}$	−0.23	−3.0
$\frac{(\delta V)_a}{A}=-\frac{n+1}{4}\frac{\langle r^2\rangle_{\text{av}}}{R_0^2}\frac{\Gamma(1+1/n)}{\Gamma(1+3/n)}\times\left[\left(\frac{3}{5}\right)^{1+1/n}a_2'\rho_0^{2/3}+\left(\frac{1}{2}\right)^{1+1/n}a_3\rho_0+\left(\frac{3}{7}\right)^{1+1/n}a_4'\rho_0^{4/3}\right]$	4.8	2.7
$\frac{(\delta V)_f}{A}=\frac{[k_F(\rho_0/2)s_0]^2}{20}\left[\frac{97-n}{100}\left(\frac{3}{5}\right)^{1+3/n}a_2'\rho_0^{2/3}+\frac{117-n}{120}\left(\frac{1}{2}\right)^{1+3/n}a_3\rho_0+\frac{137-n}{140}\times\left(\frac{3}{7}\right)^{1+3/n}a_4\rho_0^{4/3}\right]$	0.03	0.03
$\frac{E_c}{A}=\frac{3}{5}\frac{(Ze)^2}{AR_{\text{eff}}}$	3.7	3.4
E/A	−1.6	−5.7

In Table I, Column A, we show the general form of each part of E/A, using the distribution Eq. (23). The symmetry energy is not included in this calculation. It is positive and small; from the Weizsäcker semiempirical mass formula it is 0.7 Mev for $A\sim150$. In Column B we show the numerical values that are obtained for $A=150$, $Z=62$, using the empirical values of R_0 and n. The energy can be minimized by varying the trial function $\chi_i(r)$, which depends upon the two parameters R_0 and n. We have done this for $A=150$ and find an optimum binding energy of $E/A=-5.7$ Mev with $R_0=5.06$ f. and $n=2.7$.

The empirical values[12,16] are $E/A=-8.25$ Mev, $R_0=6.03$ f, and $n=6.7$. The numerical values of the individual contributions to the energy are shown in Table I, and the values of c and t, in Table II. The dependence on the mass number A, as determined from minimization of the total energy for other values of A, is in agreement with the form of Eq. (29).

One may examine our expression for the energy if R_0 and n are assumed to have their asymptotic (large-A) forms

$$R_0=r_0A^{\frac{1}{3}},\qquad n=n_0A^{\frac{1}{3}}. \tag{36}$$

The results can then be compared with the Weizsäcker semiempirical mass formula.[17] The one distinctive feature is that $(\delta V)_f/A$ is proportional to $A^{\frac{1}{3}}$; this dependence follows from the constant falloff distance which is implied by Eq. (36). It should be noted that the Weizsäcker formula is essentially an expansion in powers of $A^{\frac{1}{3}}$, which is not large for actual nuclei. Thus, there is a large ambiguity in the actual coefficients of the Weizsäcker formula and several alternative forms[17,18] have been proposed and successfully used.[19] Even the "volume energy" term, which is often used as a basis for comparison of theories of nuclear matter, differs by 1.2 Mev per particle in these various determinations. The form we have obtained might also be used to obtain a fit to the nuclear masses, since it includes the Hofstadter observations on the shape of the nuclear surface. However, it will probably not be possible to obtain a fit which is a significant improvement over those already obtained, since the number of parameters is already large and the range of $A^{\frac{1}{3}}$ is small.

TABLE II. The half-density radius c and the falloff distance t for $A=150$. Column A: empirical values[a]; Column B: results obtained by minimizing Eq. (1) using the trial function Eqs. (2) and (23); Column C: results obtained by minimizing Eq. (1), if corrections $(\delta T)_a$, $(\delta T)_f$, and $(\delta V)_a$ are reduced by 50%; Column D: results obtained by minimizing Eq. (1) including the core correction, Eq. (37).

	A	B	C	D
c(f)	5.73	4.42	4.32	3.86
t(f)	2.5	4.7	4.1	4.1

[a] R. Hofstadter, Revs. Modern Phys. **28**, 214 (1956).

IV. DISCUSSION

The results of the last section have shown that this model gives qualitative agreement with the observed binding energy and shape of nuclei, but that it fails to agree in quantitative detail. The binding energy that we find is too small, the mean square radius is too small (leading to a central density which is higher than expected), and the falloff distance is too large. We shall discuss here several possible explanations for this failure. Separately they seem inadequate to explain the discrepancy, but all are corrections which certainly should be made and which together might permit a quantitative understanding of the nuclear surface. They are (1) poor trial wave function $\chi_i(r)$, (2) breakdown of the assumption of a dependence solely on "local" density, and (3) breakdown of the "uniformity" assumption, i.e., formation of clusters.

(1) The only way to test our trial function is to compare the results which it gives with experimental data or to solve for the exact functions Ψ_i. In our particular case a comparison with experiment tests not only the wave function but the local uniformity assumption and the approximations implied by Eq. (1) (neglect of clusters, etc.) After this calculation was completed, we learned[20] that the numerical calculation proposed in II (that is, an exact calculation of Ψ_i) had been completed, also yielding too little binding ($E/A\sim-5$ Mev) and a high central density. Our large falloff distance may be attributed to a failure of our trial function.

To provide a guide to the sensitivity of our results to the wave function, one can modify various terms in the energy and determine the effect of these modifications on the energy and shape parameters. As an example, a different wave function might reduce the surface corrections. If $(\delta T)_a$, $(\delta T)_f$, and $(\delta V)_a$ were all reduced by 50%, the energy would become lower to $E/A=-7.2$ Mev, while the half-density radius would be reduced by 0.1 f and the falloff distance by 0.6 f (Table II, Column C). Hence, it appears that our results are fairly insensitive to the form of the wave function, and a quite drastic change would be required to yield the observed values.

(2) The dependence on local density appears in the variation of the K matrix with density. It is primarily the core contribution which is density dependent, becoming less repulsive as the density decreases. This has

[16] D. Strominger, in *Nuclear Spectroscopy* (Academic Press, Inc., New York, 1960), Part B.
[17] A. E. S. Green, Phys. Rev. **95**, 1006 (1954).
[18] A. G. W. Cameron, Can. J. Phys. **35**, 1021 (1957).
[19] We acknowledge a fruitful discussion with Professor W. F. Hornyak on this point.
[20] K. A. Brueckner (private communication). See also *Proceedings of the International Conference on the Nuclear Optical Model, Florida State University, Studies, No. 32*, edited by A. E. S. Green, C. E. Porter, and D. S. Saxon (The Florida State University, Tallahassee, Florida, 1959).

a simple physical interpretation: The Pauli principle requires the two-body wave function to "heal"[21] (approach its uncorrelated form) for separations of the order of the Fermi wavelength, while the hard core requires it to vanish at the core radius. As the density decreases, $\lambda\!\!\!^{-}_F$ increases and the wave function need not "heal" so rapidly, leading to less curvature in the wave function and a lower energy. This effect was included by calculating the K matrix in uniform media of various densities, as discussed earlier.

It may be, however, that the core corrections are quite different in a region where the density is varying rapidly. It would appear that the relevant parameter here is the change in density over a distance of the order of $\lambda\!\!\!^{-}_F$. If the effect of the Pauli principle upon the core contribution were diminished, more binding would result and the equilibrium shape might be different.[22]

One can use our model to estimate the magnitude of such an effect. In II it is shown that the core contribution can be approximated by

$$(\mathbf{r}|K|\mathbf{r}')_{\text{core}}=A(\rho)\delta(r-r_c)\frac{\delta(r'-r_c)}{4\pi r_c^2}, \tag{37}$$

where $A(\rho)$ decreases with decreasing density. We shall make a crude calculation of the correction to this due to variations in density, with the aim of determining the magnitude of the energy difference and its effect on the nuclear shape. To do this, we represent the correction to $A(\rho)$ by

$$\delta A(\rho)=-\frac{\lambda\!\!\!^{-}_F}{\rho}\frac{d\rho}{dR}[A^{(0)}-A(\rho_0)], \tag{38}$$

where $A^{(0)}=\hbar^2/Mr_c$ is the hard-core contribution for free particles, and $(\lambda\!\!\!^{-}_F/\rho)(d\rho/dR)$ is the fractional change in density over a Fermi wavelength (R is the center-of-mass coordinate). This has the form we expect, but its magnitude is only an arbitrary estimate. The correction to the energy has the form

$$(\delta V)_{\text{core}}=-4\pi r_c^2[\langle\bar{A}^{(0)}\rangle-\langle\bar{A}(\rho_0)\rangle]\times\int d^3R\rho^2(R)\lambda\!\!\!^{-}_F(R)\frac{d\ln\rho(R)}{dR}. \tag{39}$$

The spin-isospin averages give, including even states only,

$$\langle\bar{A}^{(0)}\rangle=\tfrac{3}{8}A^{(0)}=37.0 \text{ Mev-f.}$$
$$\langle\bar{A}(\rho_0)\rangle=\tfrac{3}{16}[A_{\text{singlet}}(\rho_0)+A_{\text{triplet}}(\rho_0)]=94 \text{ Mev-f.} \tag{40}$$

Inserting this result into the expression for the energy, we find an additional binding energy of 5.1 Mev and values of c and t given in Column D, Table II. Clearly the energy correction is of the right order of magnitude (2.5 Mev is "needed"), but the effect upon the shape is quite small. Again it would appear that quite drastic modifications in the model are required to obtain the observed, very small, falloff distance.

(3) It has been shown quite conclusively[23] that cluster effects are small in uniform nuclear matter, primarily as a result of the Pauli principle. In the surface the consequences of the Pauli principle are not as clear, and it has been suggested by many people[24] that there may be cluster formation in the surface. It is, of course, quite difficult to obtain any quantitative insight into this possibility. One might note that the binding energy per particle in a nuclear medium of even quite low density ($\sim$10 Mev according to I, excluding the Coulomb energy) is considerably larger than the binding energy per particle in an α particle (7.1 Mev). Hence, cluster formation in the nuclear surface must, if it exists, be quite different from simple formation of light nuclei; in particular, the gain in potential energy which can occur must not be overbalanced by the increase in kinetic energy, as it is in light nuclei. This is clearly a question which requires much further investigation.

[21] L. C. Gomes, D. Walecka, and V. F. Weisskopf, Ann. Phys. 3, 241 (1958).

[22] We would like to acknowledge an interesting discussion with Professor K. A. Brueckner on this point.

[23] K. A. Brueckner, Phys. Rev. **100**, 36 (1955); H. A. Bethe, Phys. Rev. **103**, 1353 (1956).

[24] For instance, D. H. Wilkinson, Phil. Mag. 4, 215 (1959).