Statistical Theory of Nuclei*

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The energy-density formalism is applied to finite nuclei. The total energy of the many-nucleon system is expressed as a functional $E(\rho)$ of the local density $\rho(r)$, and the ground-state density distribution is found by minimization with respect to $\rho(r)$. The functional of the potential energy is directly derived from a nuclear-matter calculation with variable neutron excess by Brueckner *et al.* The density-gradient correction which takes care of the density variation at the nuclear surface contains an exchange- and a correlation-energy part. In a first attempt, proton and neutron densities are assumed proportional; therefore the present calculation is limited to light nuclei. The density distributions are found to be of the so-called modified Gaussian type with a cubic polynomial. Binding energy, radius, and surface thickness are in good agreement with experiment.

I. INTRODUCTION

THE Thomas-Fermi approximation has proved to be very useful in reproducing bulk properties of the nucleus. Easier to handle than the Hartree-Fock method, the statistical theory may well serve as a starting point for nuclear-structure investigations. Remarkable results have been obtained by Gombas,[1] Skyrme,[2] and Seyler and Blanchard,[3] for instance, assuming different kinds of simple interactions between the nucleons. Their special choices of the two-body nuclear force, however, restrict somewhat the "range" of their conclusions.

In a semiphenomenological way, the Thomas-Fermi method has been applied by Berg and Wilets[4] to the study of nuclear-surface effects. They showed how even crude assumptions on the energy density of the system can yield results in qualitative agreement with experiment. Further refinements have been made by Wilets[5] and Bodmer[6] for studying details of the matter distribution.

Since it was recognized that the strongly repulsive short-range part of the nucleon-nucleon potential plays a key role in nuclear structure, attempts have been made by Hara[7] and Kumar *et al.*[8] to deal with more realistic nuclear interactions using the $\mathcal{K}$-matrix theory of Brueckner *et al.*[9] Recently, Bethe has reexamined the Thomas-Fermi theory of nuclei[10] in the same spirit, that is, in trying to remain as close as possible to the theory of nuclear matter and assuming realistic nuclear forces.

The present work is also a straightforward application of the energy-density formalism to nuclei. We express the total energy of the many-nucleon system as a functional $E[\rho]$ of the local density $\rho(r)$ and find the ground-state density distribution through minimization with respect to $\rho(r)$. Justification of this treatment can be found in the work by Kohn and collaborators.[11] The functional of the potential energy is directly derived from a nuclear-matter calculation with variable neutron excess carried out by Brueckner *et al.*[12] As far as the inhomogeneity corrections are concerned, the main part arises from the finite range of the nuclear forces. The numerical coefficient of this correction is adjusted in order to reproduce the experimental binding energy of Ca^{40}. This is the only phenomenological parameter entering into our calculation and we show that our choice is consistent with a theoretical estimate. What is more, the radii and surface thicknesses obtained are not strongly affected by this choice. The so-called Weizsäcker term with the corrected coefficient is found to be not negligible and is included. As a first step, proton and neutron densities are assumed to be proportional, so that our calculation is limited to light and medium nuclei.

In Sec. II the general method is given in some detail, together with our energy functional. Sections III and IV are devoted to the minimization procedures. Results and conclusions are presented in Sec. V.

II. ENERGY FUNCTIONAL

A complete theory of finite nuclei would require the knowledge of the nuclear two-body force as well as some appropriate treatment of the many-body system. To the extent that nuclear forces can be simulated by smooth, even nonlocal, effective interactions, it should be possible to solve the problem by using the Hartree-

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Fock approximation.[13] For realistic interactions it is known that the short-range correlations have to be treated by a ladder summation through the introduction of the $\mathcal{K}$ matrix.[9] In both cases finding the self-consistent average potential

$$\mathcal{U}(m)=\sum_{n<k_F}\langle mn|V|mn\rangle \tag{1}$$

gives rise to a tedious calculation that is hardly feasible at present, especially for heavy nuclei.

The problem for infinite nuclear matter, however, is considerably less complicated. In fact, because of translational invariance and the absence of the Coulomb energy, the state vectors are plane waves and the Hartree-Fock self-consistency problem just reduces to the definition of the single-particle energies

$$E_p=p^2/2M+\mathcal{U}(\rho). \tag{2}$$

Therefore, it would be worthwhile to make as much use as possible of nuclear-matter results in describing the finite nuclei. The statistical theory provides a natural framework for such an approach. Kohn and collaborators[11] have shown that for a quantum-mechanical system the energy can be expressed as a unique functional of the density. The exact knowledge of this very complicated and, of course, unknown functional would lead to the solution of the problem through minimization. The aim of a statistical theory is to approximate this functional in a semiclassical way. When the density is slowly varying we can expand the energy in powers of the density gradients. In this approximation, however, we lose the shell structure that can be considered as arising from the quantum oscillations created by the vanishing of the density outside the nucleus.[11] The Thomas-Fermi approximation consists in assuming that the energy dependence in the density is locally the same as that of a homogeneous medium in its ground state. This is equivalent to assuming that the correlations between the nucleons in finite nuclei are the same as in nuclear matter[9] and is known as the local-density approximation. It breaks down when the density becomes low, because then the de Broglie wavelength becomes large.

We turn now to a discussion of the individual terms in the energy functional.

A. Homogeneous Term

We have fitted the nuclear-matter saturation curves for variable neutron excess of Brueckner *et al.*[12] by the expression

$$\mathcal{T}(\rho,\alpha)+\mathcal{V}(\rho,\alpha),$$

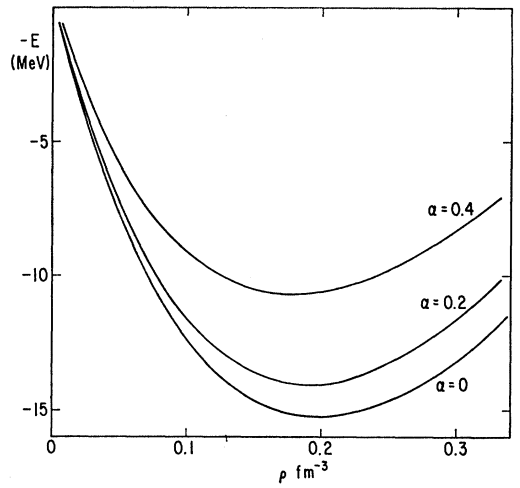

FIG. 1. Nuclear-matter saturation curves for various neutron excess. These are fitted to the results of Brueckner *et al.* (see Ref. 12).

where

$$\mathcal{T}(\rho,\alpha)\equiv C_K(\alpha)\rho^{2/3} \tag{3}$$

with

$$C_K(\alpha)=0.3(\hbar^2/M)(3\pi^2)^{2/3}\times\{[\tfrac{1}{2}(1-\alpha)]^{5/3}+[\tfrac{1}{2}(1+\alpha)]^{5/3}\} \tag{4}$$

and

$$\mathcal{V}(\rho,\alpha)=B_1(\alpha)\rho+B_2(\alpha)\rho^{4/3}+B_3(\alpha)\rho^{5/3}.$$

The coefficients $B_i(\alpha)$ are of the form $B_i(\alpha)=b_i(1+a_i\alpha^2)$. Here ρ is the total nucleon density and α is the neutron-excess parameter: $\alpha=(N-Z)/(N+Z)$. The reason for including a term linear in ρ is that at very low densities the interaction energy is proportional to the probability of having another particle in the neighborhood. Using the analytical expression (3) we were able to fit numerical points of the saturation curve[12] with a precision better than 1%. These curves are plotted in Fig. 1.

In this paper we limit ourselves to the case where the neutron and proton densities are proportional to each other throughout the nucleus. This approximation is expected to be good for medium-size nuclei. It definitely will break down for heavy nuclei in which the Coulomb energy produces an accumulation of protons near the surface. There is also strong evidence from K-capture experiments[14] that the neutron tail extends out farther than the proton tail. Work on the more general problem with independent proton and neutron densities and its application to isotope shifts and K capture is now in progress.

B. Coulomb Energy

The form of the energy density $\rho[\mathcal{T}(\rho,\alpha)+\mathcal{V}(\rho,\alpha)]$ is valid for uniform, infinite nuclear matter. For finite nuclei we have to add the Coulomb-energy term

$$C_c\rho(r)\Phi_c(r)+C_{ce}\rho(r)^{4/3} \tag{5}$$

[13] See, for instance, K. T. R. Davies, S. J. Krieger, and M. Baranger, Nucl. Phys. **84**, 545 (1966); J. P. Svenne, A. K. Kerman, and F. Villars, Phys. Rev. **147**, 710 (1966); D. M. Brink and E. Boeker, Nucl. Phys. **A91**, 1 (1967); and D. Vautherin and M. Véneroni, Phys. Letters **25B**, 175 (1967).

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with

$$C_c=\tfrac{1}{2}[\tfrac{1}{2}(1-\alpha)]e \quad \text{and} \quad C_{ce}=-1.0636[\tfrac{1}{2}(1-\alpha)]^{4/3}. \quad (6)$$

The Coulomb potential is defined as

$$\Phi_c=e\tfrac{1}{2}(1-\alpha)\int \frac{\rho(r')}{|\mathbf{r}-\mathbf{r}'|}d^3r'. \quad (7)$$

The reason for taking the direct Coulomb energy proportional to Z^2 rather than to $Z(Z-1)$ is discussed by Peaslee.[15] The small term proportional to $\rho^{4/3}$ comes from the exchange part of the Coulomb potential.[1]

C. Inhomogeneity Corrections

For a density-varying medium such as the nucleus we have to include gradient corrections to the energy density which will take the form[11]

$$\mathcal{E}[\rho]=\mathcal{E}_0(\rho)+(B_w(\rho)+B_c(\rho))(\nabla\rho)^2+\cdots. \quad (8)$$

The density-gradient correction has been separated into an exchange- and correlation-energy part. The exact form of the exchange part, arising solely from the Pauli principle and known as the Weizsäcker correction, is of the form $B_w(\rho)=(\hbar^2/8M)\xi(\nabla\rho)^2/\rho$ with $\xi=\frac{1}{9}$. It will be rederived in a very simple way in the Appendix, where we shall also motivate our particular choice of $B_c(\rho)=\eta(\hbar^2/8M)$ for the correlation-energy term. Here, η will be kept as a parameter and will be adjusted to give the correct experimental binding energies. In the present calculation, η is expressed in fm^3, whereas ξ is dimensionless.

Collecting together the various contributions, we obtain the functional to be minimized in the form

$$E[\rho]=\int \mathcal{E}[\rho(r)](dr)^3 \quad (9)$$

with

$$\mathcal{E}[\rho]=C_K\rho^{5/3}+\rho\mathcal{U}(\rho,\alpha)+C_c\rho\Phi_c+C_{ce}\rho^{4/3}+(\hbar^2/8M)\{\xi(\nabla\rho)^2/\rho+\eta(\nabla\rho)^2\}. \quad (10)$$

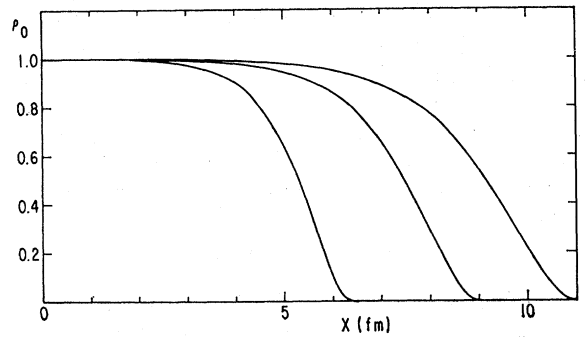

FIG. 2. Typical results for the one-dimensional nucleus for $\eta=5$, 10, and 15. The corresponding surface thicknesses are 2, 2.9, and 3.6 fm, respectively.

[15] D. C. Peaslee, Phys. Rev. **95**, 717 (1959).

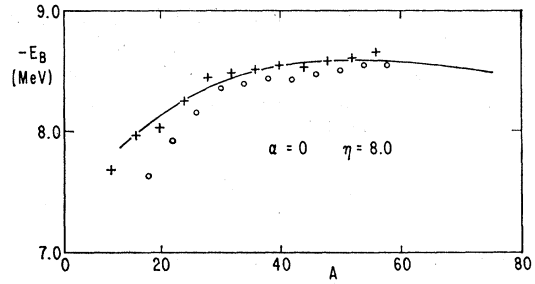

FIG. 3. Binding energy of the $\alpha=0$ nuclei obtained with the differential equation with $\eta=8$. The crosses represent the experimental values of the even-even nuclei whereas the circles correspond to odd-odd nuclei. The solid line is the theoretical curve.

III. DIFFERENTIAL EQUATION

In this section we calculate the ground-state density distribution by solving the Lagrange-type differential equation associated with (9). In other words, we seek the function $\rho(r)$ that minimizes the total energy of the many-nucleon system. Since $\rho(r)$ is subject to the condition

$$\int \rho(r)d^3r=A, \quad (11)$$

we arrive at the following second-order differential equation for the density:

$$\rho''=-\frac{2}{r}\rho'+\frac{5}{3}\frac{C_K}{2a}\rho^{2/3}+\frac{B_1}{a}\rho+\frac{7}{3}\frac{B_2}{2a}\rho^{4/3}+\frac{8}{3}\frac{B_3}{2a}\rho^{5/3}+\frac{2}{3}\frac{C_{ce}}{a}\rho^{1/3}+\frac{1}{2a}(C_c\Phi_c(r)-\mathcal{E}_0) \quad (12)$$

with

$$a=(\hbar^2/8M)\eta.$$

The origin of the terms has been explained in the previous section. For the sake of simplicity, the so-called Weizsäcker term has been neglected in the inhomogeneity correction. The Lagrange multiplier $\mathcal{E}_0$ is the binding energy of the last particle. Because of symmetry reasons, $\rho'(0)=0$, the other boundary conditions being ρ' and $\rho\to 0$ as $r\to\infty$ and $\rho(0)=\rho_0$.

Because of the Coulomb term, Eq. (12) is an integro-differential equation. It is convenient, however, to reduce it to a system of two second-order differential equations. The Coulomb potential $\Phi_c(r)$ is then given by the Poisson equation

$$\nabla^2\Phi_c(r)=4\pi e[\tfrac{1}{2}(1-\alpha)]\rho(r) \quad (13)$$

with the boundary conditions $\Phi_c(0)=\Phi_0,\Phi_c'(0)=0$ and $\Phi_c(r)\to 0$ as $r\to\infty$.

Self-consistency requires the simultaneous solution of the two differential equations, which could lead to a tedious iteration process. However, reasonable assumptions concerning the boundary value $\Phi_c(0)$ reduce the problem to a two-eigenvalue search.

TABLE I. Comparison between the solution of the differential equation for Ca^{40} and results of the variational method for modified Fermi ($n=1$) and modified Gaussian ($n=2$) distributions. These results are obtained with $\eta=6$ and $\xi=0$.

	n	p	q	R	B	$-$ (Binding energy) (MeV)	R_{eff}	T_{eff}	ρ_0
A1	1	−0.04	0	4.30	0.28	362.4	3.65	2.80	0.2235
A2	2	−0.0395	0	4.29	1.50	362.5	3.65	2.81	0.2217
A3	1	−0.016	−0.005	4.23	0.31	362.9	3.57	2.44	0.207
A4	2	0.0062	−0.01	4.25	1.70	363.2	3.64	2.11	0.194
			Differential equation			364.3	3.62	2.11	0.1993

The solution of our two coupled differential equations is by no means a simple function. Also for given ρ_0 and $\mathcal{E}_0$ values, $\rho(r)$ may well go to $\pm\infty$ or oscillate. It has been shown, however, by Kumar *et al.*[8] that the proper solution is such that $\rho(r)$ and $\rho'(r)$ vanish at some point $r=R$ and that $\rho\equiv 0$ for $r>R$. The two coupled differential equations have been solved for Ca^{40}. This nucleus has been chosen because its A is already large enough to allow a statistical treatment and probably still small enough, so that proton and neutron densities may be taken as proportional.

The results are shown in Fig. 2 and Table I for the arbitrary choice $\eta=6$. The binding energy and the surface thickness are, respectively, larger and smaller than the experimental values, whereas the half-density radius $R_{eff}=3.62$ fm is in good agreement with the empirical law $R_{eff}=1.06\times A^{2/3}$ fm. Taking $\eta=10$ lowers the binding energy to 325 MeV and raises the surface thickness to 2.70 fm without affecting the half-density radius. The experimental situation corresponds to $\eta\cong 8$. The central density ρ_0 comes out to be ≈ 0.20 fm^{-3} for $\eta=6$ and ≈ 0.19 fm^{-3} for $\eta=10$, to be compared with $\rho_0\approx 0.16$ deduced from electron scattering data; this means that the tails of our distributions extend over a shorter range.

We have also computed the binding energy per particle for the $\alpha=0$ nuclei, setting $\eta=8$. The results, plotted in Fig. 3, are in good agreement with experiment.

A usual way of simplifying the problem consists in considering a one-dimensional nucleus and neglecting the Coulomb energy. In this case Eq. (12) becomes

$$\rho''=-\frac{5}{3}\frac{C_k}{2}\rho^{2/3}+\frac{B_1}{a}\rho+\frac{7}{3}\frac{B_2}{2a}\rho^{4/3}+\frac{8}{3}\frac{B_3}{2a}\rho^{5/3}-\frac{\mathcal{E}_0}{2a}. \quad (14)$$

The integration with respect to ρ is immediate and gives

$$\rho'^2=C_k\rho^{5/3}+B_1\rho^2+B_2\rho^{7/3}+B_3\rho^{8/3}-\mathcal{E}_0\rho. \quad (15)$$

The boundary conditions imply

$$\mathcal{E}_0=C_k\rho_0^{2/3}+B_1\rho_0+B_2\rho_0^{4/3}+B_3\rho_0^{5/3} \quad (16)$$

and

$$2C_k+3B_1\rho_0^{1/3}+4B_2\rho_0^{2/3}+5B_3\rho_0=0. \quad (17)$$

Therefore, $\mathcal{E}_0$ and ρ_0 are fixed by the saturation conditions and the numerical integration of (15) is straightforward. Typical results are shown in Fig. 4 for $\eta=5$, 10, and 15. This approximation is certainly useful for comparing different saturation curves and yields qualitative results. However, it is not appropriate for actual nuclei in which the curvature effects are not negligible.

IV. VARIATIONAL METHOD

Because of the very large sensitivity of the solutions to the eigenvalues, the handling of the differential equation is rather tedious, and it is desirable to find a numerically faster way of dealing with the minimization of Eq. (9). In a variational approach to this problem, we assume a parametrized form for the density $\rho(r;\lambda_1\cdots\lambda_k)$ and search for a minimum of $E[\rho]$ within this chosen functional space.

The analytical forms we have tried are:

(A) a modified Fermi-type ($n=1$)

$$\rho(r)=\rho_0\mathcal{P}(r)\{1+\exp[(r^n-R^n)/B^n]\}^{-1}, \quad (18)$$

or a modified Gaussian ($n=2$), both with

$$\mathcal{P}(r)\equiv 1+pr^2+qr^3; \quad (19)$$

(B) a Gaussian-type

$$\rho(r)=\rho_0\mathcal{P}(r)\exp(-r^2/R^2); \quad (20)$$

(C) and finally

$$\rho(r)=\rho_0[(1+pr^2)\{1+\exp[(r-R)/B]\}]^{-1}. \quad (21)$$

The parameters to be varied are R, B, p, and q. The constant ρ_0 is determined by the condition for keeping

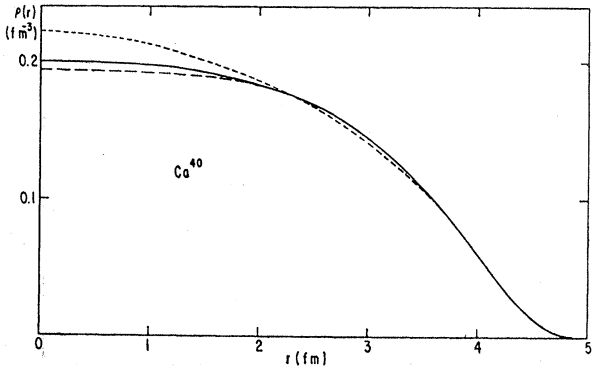

FIG. 4. Comparison between the solution of the differential equation (solid line) and those of the variational method for a modified Fermi function (short dashes) and a modified Gaussian function (long dashes) both with a cubic polynomial. Here $\eta=6$, $\xi=0$.

TABLE II. This table illustrates, in the case of Ca^{40}, the fact that the binding energy is a slowly varying function of the parameters near its minimum. E_{surf} represents the gradient correction ($\eta=6$).

		− (Binding energy) (MeV)	ρ_0	$E_{Coulomb}$	E_{surf}
Input parameters $n=2$	$R=$ 4.25 $B=$ 1.675 $p=$ 0.00625 $q=-0.01$	363.26	0.1961	87.6	80.7
$\Delta R=\pm$ 1%		363.06 363.12	0.1909 0.1995	87.1 88.1	79.1 82.4
$\Delta B=\pm$ 1.5%		363.14 363.08	0.1967 0.1903	87.6 87.1	80.2 79.4
$\Delta p=\pm$20%		363.08 363.12	0.1898 0.1985	87.1 88.1	78.6 82.9
$\Delta q=\pm$12.5%		360.34 361.44	0.2109 0.1788	89.9 85.5	83.2 77.6

the number of nucleons A fixed. The polynomial $\mathcal{P}(r)$ is set equal to zero when it becomes negative at large r to avoid having negative densities. This abrupt cutoff is, of course, unphysical since a localized quantum-mechanical system is always characterized by an exponential falloff for large r. However, we are not particularly worried about this fact, because the Thomas-Fermi energy functional breaks down anyway at small densities, where the de Broglie wavelength becomes very large. Generally, no improvement is found in fitting an exponential tail to our density curve. This is necessary, however, when the $(\nabla\rho)^2/\rho$ term is taken into account, because in this case the gradient is supposed to vanish faster than the density.

In order to check the results obtained by solving the differential equation for Ca^{40}, we omitted the Weizsäcker exchange density-gradient correction and also set $\eta=6$. We had to discard the trial functions (B) and (C) because they gave far too small binding energies. The so-called three-parameter Fermi function (A) with a quadratic polynomial did not come close to the solution of the differential equation, so we included a cubic term.

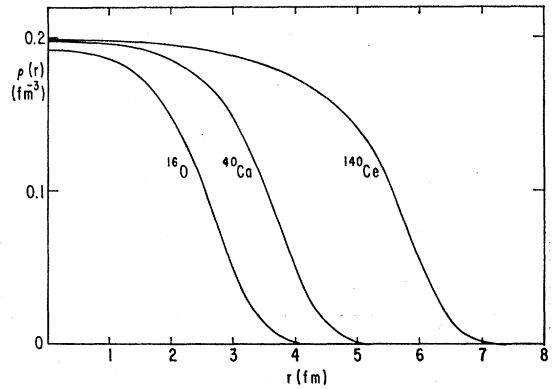

FIG. 5. Results for O^{16}, Ca^{40}, and Ce^{140} obtained from the variational method for a modified Gaussian function with a cubic polynomial. Here $\eta=5$, $\xi=\frac{1}{9}$.

The results of the variation are given in Table I. The contribution of the Coulomb energy to the binding energy lies between 87 and 88 MeV for all four distributions. The inhomogeneity contribution to energy is slightly higher for the "squarer" distributions (A3) and (A4). We have defined the effective radius (R_{eff}) as the half-density radius and the surface thickness (T_{eff}) as the 90%–10% falloff distance.

As is also seen from Fig. 5, where we plotted curves (A2) and (A4) as well as the solution of the differential equation, the curves are very close to each other for large r although the central densities are different. This comes about through the r^2 weighting factor in the radial integration. The total energy is then not very sensitive to the central density and most of the contribution comes from the surface region of the nucleus.

The results of the variational method are also compared to those of the differential equation in Table I. As far as the binding energy is concerned, the small remaining discrepancy ($\sim\frac{1}{4}$%) is attributed to the Coulomb energy. As explained in the preceding section, this is not treated self-consistently in the case of the differential equation and depends somewhat on the choice of $\Phi_c(0)$.

The binding energy is a very slowly varying function of the parameter near its minimum. In order to exhibit this effect and the precision with which we have defined the parameters, some numerical results are given in Table II.

We have performed the numerical integration using Simpson's rule with a mesh size of 151, integrating up to 3.5 times the radius parameter R. Minimization is obtained by varying one parameter while keeping the others fixed until the desired precision in all the parameters is achieved. Because of the crudeness of the integration method and the relative insensitivity of the energy, it has not seemed useful to us to increase the precision in the determination of the minimal set of parameters beyond that achieved.

Having established that the two methods give essentially the same result, we proceeded to include the Weizsäcker exchange correction $(\hbar^2/72M)(\nabla\rho)^2/\rho$. This proved to be much easier and numerically faster with the variational method. Because of the density appearing in the denominator this correction has the effect of giving a longer tail to the distribution and of reducing the binding energy by almost 40 MeV. Again the form (A) with $n=2$ and with a cubic polynomial gives a lower energy than the other trial forms. As the parameter η enters phenomenologically into our treatment we let it vary between 3 and 7. The results are given in Table III. The binding energy, as obtained from minimization of the form (A4), varies almost linearly with η in the range considered. The effective radius is practically unchanged, but the surface thickness is slightly reduced as η decreases. The optimal choice of η to give the correct experimental binding energy of 341.5 MeV was found to be $\eta\cong 5$.

The variational approach has also been applied to O^{16} and Ce^{140}. The results are not expected to be very accurate in the former case because of the small number of particles. The fact that the statistical theory yields reasonable values illustrates the existence of the mean field even in very light nuclei.

The results for O^{16}, Ca^{40}, and Ce^{140} are summarized in Table IV. In all the three cases the lowest energy has been obtained with a modified Gaussian with a cubic polynomial. The parameter η has been fixed to 5. The distributions are plotted in Fig. 3.

It is interesting to note that in the case of Ce^{140} the binding energy is too small by 4%. This could mean that bringing the binding energy into agreement with experiment requires a slow decrease of η against A. However, additional binding energy is expected to arise from relaxing the proportionality of neutron and proton densities, so that no definitive conclusions can be drawn for heavy nuclei. On the other hand, as A increases, the distributions become hollow in the center and the contribution of the second-order correction in the gradient expansion, which is found to be negligible for light nuclei, should increase.

V. CONCLUSIONS

The present investigation gives an outline of the results that may be obtained from the energy-density formalism. The calculated density distributions are in good agreement with experiment. The method would be more trustworthy for heavier nuclei than those considered here. However, in this latter case, proton and neutron densities could certainly no longer be set proportional and the whole calculation would become much more tedious. It is interesting to note that the tails of our distributions are somewhat shorter than those of the Fermi-type functions generally used in analyzing electron-scattering data. Nevertheless this result may be irrelevant since the validity of our method at very low density is not well established. It has to be pointed out that Bethe[10] also finds that his calculated distributions have a short tail or, more specifically, that, at the point of the steepest slope, ρ itself is only $\sim(0.25$ to $0.35)\times\rho_0$, whereas it is $0.5\times\rho_0$ for a Fermi distribution.

On the other hand, the shape of the nuclear surface is sensitive to the slope of the potential energy curve $v(\rho,\alpha)$. Therefore the results may differ according to what two-body force is used in the nuclear-matter calculation. Study of these effects, however, lies outside the scope of this work.

The fact that the experimental binding energy is reproduced with a reasonable value of the parameter η means essentially that the surface energy comes out correctly from the theory. On the other hand, since η has been adjusted to fit the experimental binding energy, part of it accounts for the pairing effects, which are known to be very important at the surface.

As mentioned in the previous section the two methods for finding the ground-state density are nearly equivalent. The variational approach is more adaptable and provides a simple way of studying the sensitivity of the solutions to the different parameters or, eventually, to the effect of additional terms. However one has the problem of finding a suitable trial function, and this introduces a certain arbitrariness.

The energy-density formalism provides also a simple way of deriving the mean potential $U(r)$ experienced by the last bound nucleon. Taking this mean field as the shell-model potential could be a good starting point for further developments. Such a treatment would be useful in studying deformations of the mean field or the stability of superheavy nuclei. The pairing correlations could then be introduced explicitly using the Hartree-Bogoliubov theory.

TABLE III. Results for Ca^{40} obtained with a modified Gaussian $(n=2)$ in function of η and in setting $\xi=\frac{1}{9}$.

η	−(Binding energy) (MeV)	R_{eff}	T_{eff}
3.0	362.9	3.60	1.91
5.0	341.5	3.59	2.12
7.0	317.7	3.58	2.28

TABLE IV. Results obtained for O^{16}, Ca^{40}, and Ce^{140} with a modified Gaussian $(n=2)$ taking $\eta=5.0$ and $\xi=\frac{1}{9}$. Figures in parentheses are the experimental binding energies.

	−(Binding energy) (MeV)	R_{eff}	T_{eff}
O^{16}	125.2 (127.6)	2.55	2.11
Ca^{40}	341.5 (341.5)	3.59	2.12
Ce^{140}	1126.9 (1172.7)	5.58	2.69

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APPENDIX

We sketch here a short derivation of the density-gradient corrections to the kinetic energy following the density-correlation-function method. For further details we refer to the paper of Ma and Brueckner.[16]

The energy of a system, weakly perturbed by a density-coupled interaction φ_q, can be written to lowest nonvanishing order in φ as

$$E=E^0+\tfrac{1}{2}\sum_{q\neq 0}\varphi_q\varphi_{-q}\mathfrak{F}(q,0) \tag{A1}$$

and the density response as

$$\rho_q=\mathfrak{F}(q,0)\varphi_q, \tag{A2}$$

where $\mathfrak{F}(q,\omega)$ is the full density-response function. The expression for the kinetic energy is thus

$$E_{\mathrm{KE}}=E_{\mathrm{KE}}{}^0-\tfrac{1}{2}\sum_{q\neq 0}\rho_q\rho_{-q}\mathfrak{F}_{\mathrm{KE}}{}^{-1}(q,0)+\sum_q\rho_q\varphi_{-q}. \tag{A3}$$

Assuming a slowly varying inhomogeneity, we expand the response function in powers of q:

$$\begin{aligned}\mathfrak{F}(q,0)&\equiv 1/a+bq^2+O(q^4),\\ \mathfrak{F}^{-1}(q,0)&=a-a^2bq^2+O(q^4).\end{aligned} \tag{A4}$$

Similarly, we expand the energy:

$$\begin{aligned}E[\rho]&=\int\{A(\rho(x))+B(\rho(x))|\nabla\rho(x)|^2+\cdots\}(dx)^3\\ &=A(\rho_0)+\tfrac{1}{2}A''(\rho_0)\sum_{q\neq 0}\rho_q\rho_{-q}\\ &\quad+B(\rho)\sum_{q\neq 0}q^2\rho_q\rho_{-q}+\cdots.\end{aligned} \tag{A5}$$

Identifying Eqs. (A3) and (A5) we obtain

$$B(\rho_0)=\tfrac{1}{2}a^2b. \tag{A6}$$

From the well-known free fermion gas density-response function,

$$F_0(q,0)=\frac{p_0}{2\pi^2}\left\{-1+\frac{1}{qp_0}(q^2-p_0^2)\left|\frac{q-2p_0}{q+2p_0}\right|\right\} \tag{A7}$$

we find, upon expansion and use of Eq. (A6),

$$B(\rho_0)=(\pi^2/2x)p_0{}^{-3}. \tag{A8}$$

Reintroducing $\hbar$ and M, we obtain finally for spin-$\frac{1}{2}$ fermions the result of Kompaneets and Pavlovskii,[17]

$$B(\rho_0)=(\hbar^2/72M)\rho_0{}^{-1}, \tag{A9}$$

which corresponds to $\xi=\frac{1}{9}$. This value has also been found by Moszkowski and Wilets[18] in a very similar way.

In the case of protons and neutrons, we obtain for the exchange-density-gradient correction

$$\frac{\hbar^2}{72M}\left\{\frac{1}{\rho_p}(\nabla\rho_p)^2+\frac{1}{\rho_n}(\nabla\rho_n)^2\right\}=\frac{\hbar^2}{72M}\frac{1}{\rho}(\nabla\rho)^2. \tag{A10}$$

The fact that the exchange contribution to $B(\rho)$ is proportional to $1/\rho$ could have been predicted on dimensional grounds since $\rho^{-1/3}$ is the only length associated with a noninteracting system. Weizsäcker had incorrectly given the factor $\hbar^2/8M$.

The form of the potential-energy-gradient correction is more difficult to derive. In the spirit of a simple $\mathcal{K}$-matrix theory, which is equivalent to an expansion in powers of (tk_F),[19] where t is the forward-scattering amplitude, we would expect a gradient correction of the form

$$[(\nabla\rho)^2/\rho](tk_F)\sim\rho^{-2/3}(\nabla\rho)^2. \tag{A11}$$

However, the latest investigations on the convergence of the Brueckner-Goldstone theory for nuclear matter[20] yield an expansion for the energy in powers of $(c^3\rho)$,[19] where c is the correlation length (or wave function healing distance), which is of the order of the core radius.

This leads to a gradient correction of the form $(\nabla\rho)^2$. The weakness of the long-range attractive force brings about the fact that it is the size of the core which determines the convergence of the theory. However, the gradient corrections are essentially due to the long-range force even if it is much weaker than the short-range part (a very-short-range force does not give rise to gradient corrections at all) so that the previous argument breaks down. Nevertheless we shall see that the long-range force gives the same form.

If we write the contribution of the long-range part as

$$\frac{1}{2}\int(dr)^3\rho(r)\int(dr')^3v(r')\rho(|\mathbf{r}+\mathbf{r}'|) \tag{A12}$$

and expand the density (supposed to be slowly enough varying for the gradient expansion to make sense), we

[16] S. Ma and K. A. Brueckner, Phys. Rev. **165**, 18 (1968).

[17] A. S. Kompaneets and E. S. Pavlovskii, Zh. Eksperim. i Teor. Fiz. **31**, 427 (1956) [English transl.: Soviet Phys.—JETP **4**, 328 (1957)].

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[19] V. M. Galitskii, Zh. Eksperim. i Teor. Fiz. **34**, 152 (1958) [English transl.: Soviet Phys.—JETP **34**, 104 (1958)].

[20] B. D. Day, Rev. Mod. Phys. **39**, 719 (1967); K. Rajaraman and H. A. Bethe, *ibid.* **39**, 745 (1967).

get

$$\frac{1}{2}\Big\{\int (dr)^3\rho^2(r)\int (dr')^3 v(r')+\frac{1}{2!}\int (dr)^3\rho(r)\times\sum_{ij} D_{r_ir_j}{}^2\rho(r)\int r_i'r_j'v(r')(dr')^3+\frac{1}{4!}\int (dr)^3\rho(r)\sum_{ijkl} D_{r_ir_jr_kr_l}{}^4\rho(r)\times\int r_i'r_j'r_k'r_l'v(r')(dr')^3+\cdots\Big\}. \quad \text{(A13)}$$

Making use of spherical symmetry we find

$$-\tfrac{1}{2}J_0\int (dr)^3\rho^2(r)-\tfrac{1}{12}J_2\int (dr)^3\rho\Delta\rho-\frac{1}{240}J_4\int (dr)^3\rho\Delta^2\rho+\cdots, \quad \text{(A14)}$$

where

$$J_n\equiv-\int r^n v(r)(dr)^3. \quad \text{(A15)}$$

After integration by parts the density-gradient correction becomes

$$\tfrac{1}{12}J_2\int (dr)^3(\nabla\rho(r))^2-\frac{1}{240}J_4\int (dr)^3(\Delta\rho(r))^2+\cdots. \quad \text{(A16)}$$

The first term thus gives a correction of the form $(\nabla\rho)^2$. Bethe[10] has shown that formula (A12) implies two nucleon forces separable into a long- and a short-range part and which can be written

$$V(r)=V_l(r)(1-m+mPx)+V_s(r). \quad \text{(A17)}$$

Since only the long-range part enters the calculation of η, we get

$$\eta=\frac{\pi}{4}(1-m)\int r^4V_l(r)dr. \quad \text{(A18)}$$

An additional factor $\frac{3}{4}$ has been introduced in order to account for the probability that the two nucleons have different spin or isospin or both.

As an example, we took the L_1 force of Brink and Boeker,[20] which is built up with an attractive Gaussian and repulsive δ function:

$$V(r)=V_0e^{-r^2/\mu^2}(1-m+mPx)+A\delta(r),\quad V_0=-24532,\quad \mu=0.4,\quad A=+7687,\quad m=0.5735. \quad \text{(A19)}$$

The parameters have been adjusted in order to give 15.8 MeV of binding energy per particle at $k_F=1.45$ fm^{-1} for nuclear matter and the binding energy and the size of He^4. This force is also known to yield reasonable results for O^{16} and Ca^{40}.

Inserting this force in (A18) gives $\eta=11$, which is not too far from the values we have used.

Other estimations using the $^1S_0$ part of the Reid or Hamada-Johnston potential, assuming a separation distance of 1 fm and neglecting the one-pion-exchange-potential (OPEP) contribution as suggested by Bethe,[10] yield somewhat higher values of η (~ 20–$25\hbar^2/8M$).

Finally, we would like to point out that the second-order correction of the form $\zeta(\Delta\rho)^2$ is proportional to J_4 and is even more sensitive to the range of $V_l(r)$. In the case of the L_1 force of Brink and Boeker, ζ is about 2% of η whereas it rises up to 20% in the case of the Reid potential.