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THE NUCLEAR SURFACE STUDIED WITH A MOMENTUM-DEPENDENT INTERACTION
IN THE THOMAS-FERMI AND HARTREE APPROXIMATIONS^{*}

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ABSTRACT

A self-consistent many-particle model containing a two-body interaction with a quadratic momentum dependence is developed in the Hartree approximation. The various possible algebraic forms of the momentum dependence are studied in parallel. A simple modification of the standard Thomas-Fermi approximation is formulated for the treatment of models with momentum dependent interactions. Numerical calculations are carried out for symmetric semi-infinite nuclear matter. The modified Thomas-Fermi approximation, as compared with the Hartree approximation, is found to underestimate the surface diffuseness and the surface energy by typically ten per cent. It is demonstrated that the surface properties are very sensitive to the particular algebraic form of the quadratic momentum dependence.

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1. Introduction

In this paper is studied a self-consistent many-particle model based on a two-body interaction having a quadratic momentum dependence. A general formulation is made in the Hartree approximation and the model is applied to symmetric semi-infinite nuclear matter.

The aim is to ascertain the accuracy of the Thomas-Fermi approximation for nuclear models containing a momentum-dependent interaction.

Of particular interest is the so-called Seyler-Blanchard model¹, which has been employed for several studies of macroscopic nuclear surface properties. This model is characterized by a Yukawa form of the spatial interaction, in addition to the quadratic momentum dependence; the associated many-particle problem is treated in the Thomas-Fermi approximation.

We briefly recall a few of the applications of this model. Introducing the model in 1961, Seyler and Blanchard¹ demonstrated that it reproduces the gross nuclear energetics and sizes given by experiment, for reasonable values of the few input parameters. Later on Myers and Swiatecki² adapted the model for their systematic study of macroscopic nuclear properties and they employed the model for the estimation of the coefficients entering in the Droplet Model. Recently, the model has been used to calculate the nuclear 'proximity' interaction.³

Notwithstanding the over-all qualitatively good reproduction of a variety of macroscopic nuclear properties, there remains the question of how accurate is actually the Thomas-Fermi treatment, for certain specific properties such as the matter density distribution near the surface and the surface energy coefficient.

At this point a few words of clarification should be added. The term the 'accuracy' of the treatment does not refer to a possible comparison with actual nuclei; the interest here is not in the properties of individual nuclei but in their average, macroscopic, properties. Rather, the accuracy of the Thomas-Fermi treatment is ascertained by comparing with the appropriate quantum-mechanical solution of the given many-particle problem, as it is defined by the specified two-body interaction. This is the question on which the attention is focused in this paper.

It should, of course, be explained what is meant by 'appropriate' quantum-mechanical solution. The Thomas-Fermi approximation is a classical-statistical method which treats the particles as completely independent. The present paper is concerned with the importance of the wave-mechanical nature of the particles, without giving up the assumption of complete independence. This is done in the Hartree approximation. (One can, within the framework of the Thomas-Fermi method, relax the assumption of complete independence and take account of the exchange effects due to the identity of the particles; this corresponds to the Thomas-Fermi-Dirac approximation. In a possible similar study of this approximation one should then compare with the results obtained in the Hartree-Fock approximation.) Hence, in the present investigation, the reference solution shall be that of the Hartree approximation.

First, in Section 2, the model is formulated in the Hartree approximation and the general complications arising from the momentum dependence are discussed. The specific problem of symmetric semi-infinite nuclear matter is treated in Section 3. In Section 4 the investigation is

summarized and concluded. The Appendix includes some elements of the employed formalism; this is done in order to make possible a smooth presentation.

2. Formulation of the model

The many-particle model is characterized by a specified two-body interaction V_{12} . The present study is concerned with interactions which in the classical limit reduce to the form

$$V_{12} = -C g\left(\frac{r_{12}}{a}\right) \left(1 - \frac{p_{12}^2}{b^2}\right) \quad (1)$$

Here the separation between the two interacting particles is denoted by $\vec{r}_{12} = \vec{r}_1 - \vec{r}_2$ and their relative momentum by $\vec{p}_{12} = \vec{p}_1 - \vec{p}_2$ (it is assumed that all particles have the same mass m).

The spatial dependence, assumed to possess spherical symmetry, is contained in the function g which needs not be specified yet. The Seyler-Blanchard model corresponds to the special case of g being a Yukawa function.

Only a few parameters enter: The parameter a governs the range of the interaction. The strength of the interaction decreases with increasing relative momentum in a proportion governed by the parameter b , the 'critical' momentum for which value of p_{12} the interaction changes sign. The parameter C governs the over-all interaction strength; with the minus sign exhibited, a positive value of C leads to an attractive interaction. For simplicity only one kind of particle is considered; this suffices for nuclear systems with identical neutron and proton distributions. The

generalization to two (or several) kinds of particle is straightforward; as a matter of fact, all the subsequent formulas are valid for multi-component systems provided the various density distributions entering are considered multi-component quantities and the interaction strength C is considered a matrix.

For the development of the quantum-mechanical model the interaction-energy operator corresponding to the classical interaction (1) must be specified. According to the standard rules of quantization, this is accomplished by replacing the momentum variable $\vec{p}$ in the classical interaction by the differential operator $-i\hbar\vec{\nabla}$, paying due respect to the requirement that the emerging operator be Hermitean.

The above stated general rule does not lead to a unique quantization of the classical product $p^2 g(\vec{r})$. This stems from the fact that one is not able, on any fundamental grounds, to choose between quantization prescriptions such as

$$a) \quad p^2 g(\vec{r}) \rightarrow \frac{1}{2}(p^2 g(\vec{r}) + g(\vec{r}) p^2)$$

or

$$b) \quad p^2 g(\vec{r}) \rightarrow \vec{p} g(\vec{r}) \vec{p}$$

(2)

or any combination of a) and b); they are all Hermitean and reduce to (1) in the classical limit.

Thus, there is no unique way of 'quantizing' the classical product $p^2 g(r)$. Rather, there exists a whole family of quantum-mechanical operators which all have the same classical limit. This family of operators may be parametrized by one real parameter η since all of the algebraic constructions mentioned above may be reduced to the form

$$p^2 g(\vec{r}) + \frac{1}{2} \{ \vec{p}, \frac{1}{2} \{ \vec{p}, g(\vec{r}) \} \} - \eta \frac{1}{2} [\vec{p}, \frac{1}{2} \{ \vec{p}, g(\vec{r}) \}] \quad (3)$$

Here the sharp brackets denote the commutator, $[a, b] = ab - ba$, and the curly brackets the anti-commutator, $\{a, b\} = ab + ba$.

This unified formulation makes it possible to discuss in parallel the whole family of different quantum interactions. In by-passing it should be noted that the particular algebraic forms a) and b) above are obtained for $\eta = -1$ and $\eta = +1$, respectively; for $\eta = 0$ the average of a) and b) is obtained.

Having now clarified the problems associated with the quantization, we pass on to the general formulation of the quantum-mechanical model.

The fundamental quantity in the model is the two-particle interaction-energy density operator which shall be denoted by $\hat{w}(\vec{r}', \vec{r}'')$. This operator depends on the two spatial points $\vec{r}'$ and $\vec{r}''$; in the Appendix are included some details on the formalism. The symbol $\hat{}$ is placed over a quantity to indicate that it is an operator, in cases where there could otherwise be confusion.

For the type of model studied in this paper, the two-particle interaction-energy operator is given by

$$\begin{aligned} \hat{w}(\vec{r}', \vec{r}'') = & -C g \frac{r}{a} \sum_{ij} (\delta(\vec{r}' - \vec{r}_i) \delta(\vec{r}'' - \vec{r}_j)) \\ & - \frac{1}{2} \left\{ \frac{\vec{p}_{ij}}{b}, \frac{1}{2} \left\{ \frac{\vec{p}_{ij}}{b}, \delta(\vec{r}' - \vec{r}_i) \delta(\vec{r}'' - \vec{r}_j) \right\} \right\} \\ & + \eta \frac{1}{2} \left[\frac{\vec{p}_{ij}}{b}, \frac{1}{2} \left[\frac{\vec{p}_{ij}}{b}, \delta(\vec{r}' - \vec{r}_i) \delta(\vec{r}'' - \vec{r}_j) \right] \right] \end{aligned} \quad (4)$$

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The subscript η has been attached to $\hat{w}$ to remind of the fact that the operator depends on the actual choice of the parameter η . The separation between the two spatial points is denoted by $\vec{r} = \vec{r}' - \vec{r}''$, and $\vec{p}_{ij} = \vec{p}_i - \vec{p}_j$ is the relative momentum of the two particles i and j .

From the operator $\hat{w}$ the two-particle interaction-energy density w itself is obtained by forming the expectation value with respect to the actual state of the many-particle system. This leads to

$$w_{\eta}(\vec{r}', \vec{r}'') = -C g\left(\frac{r}{a}\right) \left(\rho(\vec{r}') \rho(\vec{r}'') + 2 \vec{\pi}(\vec{r}') \cdot \vec{\pi}(\vec{r}'') - \rho(\vec{r}') \gamma(\vec{r}'') - \gamma(\vec{r}') \rho(\vec{r}'') - \eta \frac{\hbar^2}{b^2} \frac{1}{4} \Delta(\rho(\vec{r}') \rho(\vec{r}'')) \right) \quad (5)$$

where the Laplace operator Δ acts with respect to $\vec{r}$. The one-particle density distributions entering are the matter density ρ , the momentum density $\vec{\pi}$, and the kinetic density γ (which is *not* the standard kinetic-energy density). In the Appendix is given the precise definitions of these quantities.

The usual one-particle interaction-energy density, denoted by $v(\vec{r})$, is obtained by integrating $\frac{1}{2} w(\vec{r}', \vec{r}'')$ over one spatial variable,

$$v(\vec{r}) = -\frac{1}{2} C \left(\rho(\vec{r}) \mathcal{R}(\vec{r}) + 2 \vec{\pi}(\vec{r}) \cdot \vec{\mathcal{P}}(\vec{r}) - \rho(\vec{r}) \mathcal{G}(\vec{r}) - \gamma(\vec{r}) \mathcal{R}(\vec{r}) - \eta \frac{\hbar^2}{b^2} \left(\rho(\vec{r}) \Delta \mathcal{R}(\vec{r}) - 2 \vec{\nabla} \rho(\vec{r}) \cdot \vec{\nabla} \mathcal{R}(\vec{r}) + \Delta \rho(\vec{r}) \mathcal{R}(\vec{r}) \right) \right) \quad (6)$$

The functions obtained by folding the density distributions ρ , $\vec{\pi}$ and γ by the two-body interaction g are denoted by $\mathcal{R}$, $\vec{\mathcal{P}}$ and $\mathcal{G}$, as explained in the Appendix. The total interaction energy in the system is given by the integral of $v(\vec{r})$ over all space.

The operator $\hat{W}$ representing the total interaction energy is obtained by integrating $\frac{1}{2}\hat{w}(\vec{r}', \vec{r}'')$ over both spatial variables. (This leads to

$$\hat{w}_\eta = -\frac{1}{2}C \sum_{ij} \left(g\left(\frac{\vec{r}_{ij}}{a}\right) - \frac{1}{2} \left\{ \frac{\vec{p}_{ij}}{b}, \frac{1}{2} \left\{ \frac{\vec{p}_{ij}}{b}, g\left(\frac{\vec{r}_{ij}}{a}\right) \right\} \right\} - \eta \frac{\hbar^2}{b^2} (\Delta g) \left(\frac{\vec{r}_{ij}}{a}\right) \right) \quad (7)$$

where the function Δg denotes the Laplacian derivative of the function g .

In the Hartree approximation, it is possible to introduce for each individual particle an effective one-particle operator $\hat{V}^{\text{eff}}$ representing the combined interaction with the rest of the particles. For the present two-body interaction, the effective one-particle interaction operator is given by

$$\hat{V}_\eta^{\text{eff}} = -C \left(\mathcal{R} + \left\{ \frac{\vec{p}}{b}, \mathcal{P} - \mathcal{G} - \frac{1}{2} \left\{ \frac{\vec{p}}{b}, \frac{1}{2} \left\{ \frac{\vec{p}}{b}, \mathcal{R} \right\} \right\} - \frac{\hbar^2}{b^2} \Delta \mathcal{R} \right) \right) \quad (8)$$

where $\mathcal{R}$, $\mathcal{P}$ and $\mathcal{G}$ are functions of the particle position and $\vec{p}$ is the particle momentum operator. Addition of the operator $\hat{V}^{\text{eff}}$ to the particle kinetic-energy operator $\vec{p}^2/2m$ leads to the effective single-particle Hamiltonian $\hat{H}^{\text{eff}}$ governing the motion of the individual particle in the many-particle system.

For a system with $\vec{\mathcal{P}} \equiv \vec{0}$ (static system), the effective Hamiltonian may be written on the form

$$\hat{H}_\eta^{\text{eff}} = \frac{1}{2} \left\{ \vec{p}, \frac{1}{2} \left\{ \vec{p}, \frac{1}{2B} \right\} \right\} + U_\eta \quad (9)$$

i.e. in terms of a variable mass B and a static potential U .

The effective mass B is given by the relation

$$\frac{1}{2B(\vec{r})} = \frac{1}{2m} \left(1 + \frac{c}{b^2/2m} \mathcal{R}(\vec{r}) \right) \quad (10)$$

The renormalization of the particle mass arises from the quadratic momentum dependence of the integration. The effective mass B does not depend on η , i.e. on which actual algebraic quantization form is chosen. The effective potential U is given by

$$U(\vec{r}) = -c \left(\mathcal{R}(\vec{r}) - \mathcal{G}(\vec{r}) - \eta \frac{\hbar^2}{b^2} \Delta \mathcal{R}(\vec{r}) \right) \quad (11)$$

It should be pointed out that while the choice of another algebraic form of the kinetic term in the effective Hamiltonian (9) would not affect the effective mass B as given by (10), it would lead to a modification of the effective potential U . For example, if the form $\vec{p} \frac{1}{2B} \vec{p}$ were chosen instead in (9), then the function $\mathcal{G}$ in the formula (11) for U would be replaced by the function $\mathcal{I}$ (see the Appendix for definition). A simple feature of the effective Hamiltonian (9) is that it does not depend on which particle is considered; the functions B and U are common to all the particles.

The η -dependent term introduces an explicit sensitivity to density inhomogeneities. For negative values of η such inhomogeneities will raise the energy and the term will have the effect of smearing out the inhomogeneities. For positive values of η , however, the energy will be lowered by inhomogeneities and the η -dependent term will tend to enhance them. As we shall see in detail, this may prevent the existence of a self-consistent solution.

2.1 MODIFIED THOMAS-FERMI APPROXIMATION

The general properties of the self-consistent solution, considered as a function of the parameter η , can be understood from an analysis based on the Thomas-Fermi approximation.

The standard Thomas-Fermi approximation, as employed in the Seyler-Blanchard model¹, does not distinguish between the various η values and is consequently at best only a good approximation for a narrow range of η values. Below is formulated a simple modification⁴ of the standard Thomas-Fermi approximation which extends the applicability to all η values.

In eqs. (9) and (11) the effective single-particle Hamiltonian has been cast into a form which employs the double-anti-commutator for the terms originating from the momentum dependence. It can be shown⁵ that this particular algebraic form tends to average out possible phase correlations present. The presumption is now made that the Thomas-Fermi approximation is most accurate for the reproduction of these quantities. This identification between the usual Thomas-Fermi quantities and those Hartree quantities given by the double-anti-commutator form leads to the isolation of an η -dependent term by which the standard Thomas-Fermi formulas should be modified.

The effective static potential is henceforth given by

$$U_{\eta}^{TF} = U_0^{TF} + \eta \, c \, \frac{\hbar^2}{b^2} \Delta \mathcal{R}^{TF} \quad (12)$$

Here U_0^{TF} is the standard Thomas-Fermi potential given by

$$U_0^{TF} = -c(\mathcal{R}^{TF} - \mathcal{G}^{TF}) \quad (13)$$

-11-

with $\mathcal{R}^{\text{TF}}$ and $\mathcal{G}^{\text{TF}}$ generated from the Thomas-Fermi matter and kinetic distributions, respectively. Furthermore, the interaction-energy density v is modified by the additional term

$$\eta \delta v = \eta \frac{1}{2} c \frac{\hbar^2}{b^2} \frac{1}{2} \left(\rho \Delta \mathcal{R} - 2 \vec{\nabla} \rho \cdot \vec{\nabla} \mathcal{R} + \Delta \rho \mathcal{R} \right) \quad (14)$$

With this modification of the Thomas-Fermi approximation, each member of the η -family of Hartree models can be assigned a Thomas-Fermi counterpart. In the following Section, this modified approximation is employed for a study of semi-infinite nuclear matter, and quantitative comparisons are made with the Hartree approximation.

3. Application to the nuclear surface.

The attention is now turned to the nuclear surface. The following studies are carried out for the case where the spatial dependence of the two-body interaction is a Yukawa function, $g(r) = \exp(-r)/r$. This corresponds to the type of interaction introduced by Seyler and Blanchard¹. For the three model parameters entering are chosen the values determined by Myers and Swiatecki² in their study of average nuclear properties,

$$\begin{aligned} a &= 0.62567 \text{ fm} \\ b &= 372.48 \text{ MeV/c} \\ C &= 328.61 \text{ MeV} \end{aligned} \quad (15)$$

Only symmetric matter is considered, hence only the average interaction strength C is required. It should be added that the substance of the conclusions is not expected to depend either on the specific choice of a Yukawa spatial dependence or on the actual parameter values, as long as

they are reasonable.

The properties of the nuclear surface are studied by considering a semi-infinite system. In such case the calculational problem reduces effectively to one dimension, the direction perpendicular to the surface plane. Moreover, the transverse integration reduces the Yukawa function to an exponential, which is particularly simple to treat numerically. The self-consistent equilibrium solution to the many-particle problem is found by iteration, using approximate effective mass and potential functions B and U to solve for the approximate one-particle density distributions ρ and γ , which in turn are used to generate new effective potential functions B' and U' . In a Thomas-Fermi type approximation, the densities are obtained directly from the effective potential functions by means of the relation $E_F = P_F^2/2B + U$ which gives the local Fermi momentum $P_F(\vec{r})$. In the Hartree approximation, the densities are given in terms of the single-particle wave functions which are obtained by solving the effective Schrödinger equation. For this time-consuming process, a relatively fast Taylor-expansion method has been developed, obtained by successive differentiation of the Schrödinger equation; it has the advantage of being easy to check for accuracy.

3.1 THE DEPENDENCE ON η

3.1a. *Results in the modified Thomas-Fermi approximation*

On the basis of the modified Thomas-Fermi approximation formulated above, it is easy to understand the general behavior of the self-consistent solution, considered as a function of the parameter η :

For the semi-infinite system the essential degree of freedom is

associated with the surface diffuseness. As a function of the diffuseness, the part of the energy arising from the η -independent part of the interaction has a minimum at a certain diffuseness, the equilibrium diffuseness in the case of vanishing η . For the non-vanishing values of η , there is an additional energy contribution, proportional to η for a given system. The term multiplying η is negative; it tends to zero for very diffuse systems and to minus infinity for systems with very sharp surfaces. Hence, for negative η values, the additional term gives rise to an increase of the surface energy. Furthermore, it follows that the diffuseness equilibrium value is shifted towards larger values. It is worthwhile noticing that an equilibrium always exists for negative η . In the opposite case, $\eta > 0$, there is a negative contribution from the η -dependent term. For sufficiently small η values, the addition of the above-mentioned diverging function to the original function pertaining to $\eta = 0$ will still result in a function having a local minimum (as well as a maximum). The value at the minimum as well as the corresponding diffuseness will be decreased relative to the case of $\eta = 0$. However, as is evident in this simple picture, for positive η values above a certain critical value the minimum disappears and no self-consistent solution exists.

These simple qualitative considerations are borne out by actual calculations, as is illustrated in Figs. 1 - 3.

In Fig. 1 is shown, as a function of η , the surface diffuseness of the equilibrium matter density ρ . As well the 10-90% diffuseness t_{10-90} as the second surface moment $b^{6,7}$ are displayed. One observes the general decrease of the surface diffuseness as the parameter η is increased. Moreover, it appears that the critical η value in this modified Thomas-Fermi treatment lies just a little above $\eta = 0.5$.

Fig. 2 is a corresponding plot of the surface energy coefficient a_s . The general decrease of a_s with increasing η is evident as well as the collapse a little above $\eta = 0.5$.

Fig. 3 is a plot of the surface energy versus the surface diffuseness. The circles indicate the locations of the equilibrium solutions presented in Figs. 1 and 2; the corresponding η values are indicated. This figure also displays the two curves referred to in the preceding qualitative discussion, namely the η -independent part of the surface energy, a_s^0 , and the contribution δa_s from the term multiplying η . The first curve is to a very good approximation identical to what would result from a simple scaling (stretching or compression) of the equilibrium solution corresponding to $\eta = 0$; this fact underscores the close relation between the surface diffuseness and the freedom associated with the η parameter. In this figure is also shown parts of the surface-energy curves for a few non-vanishing η values. Finally it should be added that the results for η values larger than 0.5 are less accurate and are indicated by dashed lines.

3.1b *Comparison with the Hartree approximation*

The self-consistent solution has been calculated in the Hartree approximation, for $\eta = -1.0, -0.5, 0.0$, and 0.5 . Figure 4 displays the resulting matter density distributions; the corresponding Thomas-Fermi densities are indicated by dashed lines. The extracted values for the surface diffuseness and the surface energy are indicated in Figs. 1-3 by crosses.

The general trend given by the modified Thomas-Fermi analysis is well reproduced on the whole by the Hartree calculation. In particular, the results indicate that no Hartree solution exists for η values appreciably above 0.5. (Because of the associated delicate numerical problems no large computational effort has been made to determine accurately the

critical η value; it is expected to depend on the actual values of the model parameters a , b and C .)

The 10-90% surface diffusenesses obtained in the Hartree calculations are somewhat larger than the corresponding Thomas-Fermi values. This is mainly due to the density tail extending into the classically forbidden region outside the surface. This effect becomes particularly noticeable for positive η values when the Thomas-Fermi diffuseness approaches zero. For comparison is indicated the Hartree value for t_{10-90} corresponding to an infinitely sharp potential wall. For large negative values of η , where the system becomes more and more diffuse, the geometric properties of the surface profile will scale with the diffuseness. Hence the absolute discrepancy between the Thomas-Fermi value and the Hartree value for t_{10-90} will increase while the ratio will tend to a constant value. For $\eta = 0$ the relative underestimation is 10.4% and for $\eta = -1$ it is 3.2%.

The surface moment $b^{6,7}$ also follows the trend of the modified-Thomas-Fermi solutions. For positive η values it is difficult to extract an accurate b value because of the appreciable density undulations. It should be added here that the definition of the b value is not entirely well-defined for a Hartree system; this problem will be discussed later on. In general the agreement is closer for the b values than for the t_{10-90} values. This is mostly an effect of the particular quantum phasing near the surface: in the region around the inside part of the first density ripple the contribution to the surface moment is relatively small (for positive η values it is even negative); this counteracts the excess build up from the region further out.

For the surface energy (Fig. 2) there is also general agreement as to the dependence on η . The modified Thomas-Fermi approximation under-

estimates the surface energy, and increasingly so with increasing η . For $\eta = -1$ the discrepancy amounts to 3.6% and for $\eta = 0$ to 9.7%. A more detailed analysis will be carried out below, for the particular case of $\eta = 0$. The Hartree results for the surface energy are included in Fig. 3.

3.2 RESULTS FOR $\eta = 0$

After having discussed the general dependence on the η parameter, we turn now to a more detailed discussion of an individual solution. The discussion is carried through for the particular value $\eta = 0$; similar discussions would apply to other η values.

3.2a *The matter density distribution*

In Fig. 5 is shown the matter density distribution obtained for $\eta = 0$ (same as is part of Fig. 4). In the bulk region the scale has been enlarged in order to exhibit the undulations of the density.

These density undulations require special attention. In their study of nuclear density oscillations, Thorpe and Thouless⁸ show that asymptotically the density oscillations pertaining to a diffuse semi-infinite potential are essentially only modified by an overall phase shift relative to the infinite-wall oscillations. Furthermore, they state that for the diffuse potential the first density hump may drop from its infinite-wall value of 8.6% to as little as 1.6% above the Thomas-Fermi density.

The fact that the asymptotic behavior does not depend on the detailed shape of the surface profile has bearing on the applicability of surface moments for the description of semi-infinite leptodermous density profiles, along the lines suggested by Süssmann⁶ for finite nuclei. Süssmann⁶ has

advocated the idea that the nuclear density profile be described in terms of surface moments of the density distributions, the surface diffuseness being given in terms of the second moment, the surface skewness (flare) in terms of the third moment, and so on. Any two distributions may then be compared by comparing their respective surface moments. However, as was noted above, asymptotically the density amplitudes follow those pertaining to an infinite wall, which are inversely proportional to the square of the depth. Consequently all higher moments, from the second and up, are not mathematically well defined. In fact, they all exhibit an oscillatory behavior as function of the lower limit of the integral, the corresponding amplitude being constant for the second moment, increasing linearly for the third moment, and so on. Hence it is not possible to directly extract the surface-moment information about a semi-infinite quantum density distribution. For real nuclei, of course, the problem does not occur because of the finite size. But it is of general interest to study semi-infinite systems. And since this type of density ripple is a quite general feature in a Hartree description of such systems, it would be desirable to generalize the concept of surface moments to cover this case as well. Such a generalization could conceivably be brought about by defining some appropriate averaging procedure by which the convergence would be ensured. In doing so one might benefit from the knowledge of the behavior of the ripples in the asymptotic limit.

A very rough attempt along such lines has been done for the second surface moments b displayed in Fig. 1 by simple graphical averaging of the integral as function of its lower limit. Such a procedure appears relatively reliable for the second moment and the result can be compared

with the Thomas-Fermi value. But for the higher moments the development of a rigorous mathematical prescription is required.

3.2b *The kinetic densities*

The kinetic density γ obtained for $\eta = 0$ is displayed in Fig. 6. In addition is also displayed the density δ , which is what should be added or subtracted in order to obtain the 'velocity-squared' density κ or the standard kinetic-energy density τ , respectively.

It should be noted that γ has a very smooth behavior as compared with either κ or τ . This is in accordance with the general results obtained by Gräf⁵ with the generalized Thomas-Fermi approximation introduced by Swiatecki⁹.

In the tail region the kinetic-energy density τ is negative while κ remains positive. The density γ also remains positive but tends rapidly to zero, in agreement with the analysis by Gräf⁵.

The dashed line indicates the Thomas-Fermi kinetic density. It is evident from the figure that the kinetic density γ is the one best reproduced by the Thomas-Fermi kinetic density. This supports the specific modification of the Thomas-Fermi approximation formulated above.

3.2c *The surface-energy density*

We turn now to the discussion of the distribution of surface energy, as obtained in the Hartree model, for $\eta = 0$. The surface energy represents the binding-energy deficit due to the surface. Thus the surface-energy density ϵ_s is given by

$$\epsilon_s(x) = \epsilon(x) - \frac{\epsilon_0}{\rho_0} \rho(x) \quad (16)$$

where $\epsilon(x)$ is the total energy density and $\rho(x)$ the matter density, at the depth x . The corresponding asymptotic bulk values are denoted by ϵ_0 and ρ_0 . The surface energy itself is obtained as the integral of ϵ_s .

In Fig. 7 is shown the calculated surface-energy density together with the one pertaining to the Thomas-Fermi system. Figure 8 shows the decomposition of these densities into their kinetic and interaction parts. For the Hartree system those latter partial densities exhibit oscillations in the deeper part of the system. They are opposite to each other so that the combined density $\epsilon_s(x)$ has somewhat smaller oscillations. The Thomas-Fermi densities all go to zero at the endpoint while the Hartree densities extend out in the tail region. It is noted that in this region the two parts tend to cancel each other resulting in a rather negligible, slightly negative, value of the total surface-energy density.

The kinetic-energy contribution to the surface-energy density is negative (apart from the small bulk oscillations). Its behavior in the tail region reflects the fact that it is advantageous for a particle to be in this region as it has here small or even negative kinetic energy. Further inside the system the Hartree contribution is less negative than the Thomas-Fermi contribution. This is due to the quantum localization effect which prohibits low-momentum particles from getting as close to a potential wall as high-momentum particles. This exclusion of the low-momentum particles from the potential surface results in a relative excess of high-momentum particles and a corresponding higher kinetic energy in that region. In the Thomas-Fermi approximation, with its phase averaging, this effect is not taken into account. In the extreme case of a sharp wall, the kinetic-energy contribution to the surface

energy would be positive; the fact that it remains negative in the actual case is due to the diffuseness of the surface.

The interaction-energy contribution to the surface-energy density follows more closely the Thomas-Fermi curve, with some wiggles reflecting the matter-density oscillations relative to the Thomas-Fermi density. For example, the fact that ϵ_s^{int} is smaller than the Thomas-Fermi curve on the inside slope (around $-3a$) is a consequence of the first density hump which brings the density closer to the ideal bulk value and consequently lowers the energy deficit. In the tail region there is an appreciable contribution because the particles here are not very well bound. As we noticed (and this is in general true for all values of the parameter η), it so happens that this contribution to a large extent cancels the kinetic-energy gain in the tail.

The curve for the total surface-energy density then follows relatively well the Thomas-Fermi curve. The largest deviation occurs near the peak and from the discussion above it follows that this increase should be mainly ascribed to the lack of low-momentum particles near the quantum surface.

4. Summary and conclusions

In the Hartree approximation, a general formulation has been made of a many-particle model with an interaction having a quadratic momentum dependence. The various possible algebraic forms of the quadratic momentum dependence give rise to a family of related but different interactions which are studied in parallel. These interactions differ by amounts proportional to the Laplacian derivative of the spatial two-body interaction.

Thus, in the case of a Yukawa function, the difference amounts to a renormalization of the momentum independent part of the interaction together with the addition of a δ -function interaction.

A simple modification of the standard Thomas-Fermi approximation was formulated for the treatment of the momentum-dependent interactions. The modification amounts to the addition of a potential term which is proportional to the second derivative of the static potential generated by the spatial interaction. With this modification one can, within the framework of the Thomas-Fermi approximation, understand qualitatively well the general character of the self-consistent many-particle states. In particular, the Thomas-Fermi analysis indicates that for certain forms of the momentum dependence, no self-consistent solution exists.

Numerical studies were carried out for symmetric semi-infinite nuclear matter, by use of interactions similar to the widely used Seyler-Blanchard¹ interaction. A summary of the results for the surface diffuseness t_{10-90} and the surface energy a_s is presented in Table 1. Generally, the results obtained with the modified Thomas-Fermi approximation agree relatively well (typically to within ten per cent) with the Hartree results. The surface diffuseness as well as the surface energy are somewhat underestimated by the Thomas-Fermi treatment. For the surface diffuseness, this is mainly a consequence of the absence of a density tail. The underestimation of the surface energy can (for the main part) be traced to the neglect of the phase correlations in the surface region.

A particularly detailed discussion was carried through for the special case of $\eta = 0$, which, according to the connection prescription introduced alongside with the modified Thomas-Fermi approximation,

corresponds to the Seyler-Blanchard model¹. It was found that the Seyler-Blanchard model¹, with the parameter values determined by Myers and Swiatecki², underestimates the surface diffuseness t_{10-90} by 10.4% and the surface energy by 9.7%, as compared with the corresponding Hartree results.

In conclusion the following can be stated. In the nuclear case, the particular algebraic form of the momentum dependence of the two-body interaction has a large bearing on the surface properties of the corresponding self-consistent many-particle solution; this is underscored by the fact that for certain (not extreme) forms no solution exists. With a simple modification, the Thomas-Fermi approximation can be used for the treatment of many-particle systems with (quadratically) momentum-dependent interactions. This extends appreciably the applicability of the Thomas-Fermi approximation for the study of nuclear properties.

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Appendix

In this Appendix is included some elements of the formalism employed in the present study. This is done in order to make possible a smooth presentation. For simplicity, it is assumed that all particles in the many-particle system have the same mass m .

Matter density

The matter density distribution $\rho(\vec{r})$ measures, in units of m , the amount of matter located at the spatial position $\vec{r}$. It is represented by the operator

$$\hat{\rho}(\vec{r}) = \sum_i \delta(\vec{r} - \vec{r}_i) \quad (\text{A-1})$$

when $\vec{r}_i$ denotes the position of particle i . (The density distribution itself is obtained as the expectation value of this operator.)

Momentum density

The momentum density distribution $\vec{\pi}(\vec{r})$ is represented by the operator

$$\hat{\vec{\pi}}(\vec{r}) = \sum_i \frac{1}{b} \{ \vec{p}_i, \delta(\vec{r} - \vec{r}_i) \} \quad (\text{A-2})$$

Here $\vec{p}_i = -i\hbar\vec{\nabla}$ denotes the momentum operator for particle i . The anti-commutator construction has been employed to ensure Hermiticity. For convenience, the momentum is measured in units of the parameter b entering the particular type of interaction under study (1).

Kinetic densities

The kinetic-energy density distribution $\tau(\vec{r})$ is represented by the operator

$$\hat{\tau}(\vec{r}) = \sum_i \frac{1}{b^2} \{ \vec{p}_i^2, \delta(\vec{r} - \vec{r}_i) \} \quad (\text{A-3})$$

The energy unit is $\frac{b^2}{2m}$.

Another kinetic density distribution is $\kappa(\vec{r})$ represented by

$$\hat{\kappa}(\vec{r}) = \sum_i \frac{\vec{p}_i}{b} \delta(\vec{r} - \vec{r}_i) \frac{\vec{p}_i}{b} \quad (A-4)$$

It corresponds to a 'velocity-squared' density and is non-negative everywhere.

The average, $\gamma(\vec{r})$, of the above two distributions is of particular interest. It is represented by

$$\hat{\gamma}(\vec{r}) = \sum_i \frac{1}{2} \left\{ \frac{\vec{p}_i}{b}, \frac{\vec{p}_i}{b}, \delta(\vec{r} - \vec{r}_i) \right\} = \frac{1}{2} (\hat{\kappa}(\vec{r}) + \hat{\tau}(\vec{r})) \quad (A-5)$$

The following relations are elementary to prove,

$$\hat{\tau}(\vec{r}) + \delta(\vec{r}) = \hat{\gamma}(\vec{r}) = \hat{\kappa}(\vec{r}) - \delta(\vec{r}) \quad (A-6)$$

with

$$\delta(\vec{r}) = \frac{1}{2} (\hat{\kappa}(\vec{r}) - \hat{\tau}(\vec{r})) = \frac{1}{2} \frac{\hbar^2}{b^2} \Delta \phi(\vec{r}) \quad (A-7)$$

The various kinetic density distributions may be written on the general form

$$\hat{\gamma}_\eta(\vec{r}) = \hat{\gamma}(\vec{r}) - \eta \sum_i \frac{1}{2} \left[\frac{\vec{p}_i}{b}, \frac{\vec{p}_i}{b}, \delta(\vec{r} - \vec{r}_i) \right] \quad (A-8)$$

where η is a real parameter. It is noted that $\tau = \gamma_{\eta=-1}$, $\kappa = \gamma_{\eta=1}$, and

$$\gamma = \gamma_\eta = 0.$$

Folded functions

It is helpful to introduce a simple notation for the functions obtained when the various density distributions defined above are folded

with the spatial two-body interaction $g(\vec{r})$. For this, capital script letters are used. Thus, for example, the function $\mathcal{R}$ is given by

$$\mathcal{R}(\vec{r}) = \int g(\vec{r} - \vec{r}') \rho(\vec{r}') d^3\vec{r}' \quad (\text{A-9})$$

The functions $\mathcal{P}$, $\mathcal{T}$, $\mathcal{K}$, $\mathcal{G}$, and $\mathcal{D}$ are defined analogously in terms of the densities π , τ , κ , γ , and δ . Since the folding commutes with differentiation, the following relations hold,

$$\mathcal{T}(\vec{r}) + \mathcal{D}(\vec{r}) = \mathcal{G}(\vec{r}) = \mathcal{K}(\vec{r}) - \mathcal{D}(\vec{r}) \quad (\text{A-10})$$

with $\mathcal{D} = \frac{1}{2} \frac{\hbar^2}{b^2} \Delta \mathcal{R}$.

Two-body interaction

The basic quantity is the operator $\hat{w}(\vec{r}', \vec{r}'')$ representing the energy contribution arising from the interaction of particles at $\vec{r}'$ with particles at $\vec{r}''$. It is of the form

$$\hat{w}(\vec{r}', \vec{r}'') = \frac{1}{2} \sum_{ij} \hat{w}_{ij}(\vec{r}', \vec{r}'') \quad (\text{A-11})$$

where $\hat{w}_{ij}(\vec{r}', \vec{r}'')$ represents the contribution from the interaction between the particles i and j .

The total interaction energy is given by

$$W = \frac{1}{2} \iint \hat{w}(\vec{r}', \vec{r}'') d^3\vec{r}' d^3\vec{r}'' \quad (\text{A-12})$$

where w is the expectation value of $\hat{w}$. The quantity W is represented by the total interaction-energy operator

$$\hat{W} = \frac{1}{2} \iint \hat{w}(\vec{r}', \vec{r}'') d^3\vec{r}' d^3\vec{r}'' = \frac{1}{2} \sum_{ij} \hat{W}_{ij} \quad (\text{A-13})$$

where $\hat{W}_{ij}$ represents the total interaction between the particles i and j .

The usual one-particle interaction-energy density $v(\vec{r})$, which is the energy contribution due to particles located at the position $\vec{r}$, may be obtained from the two-particle density $w(\vec{r}', \vec{r}'')$ by integration over either one of the spatial variables,

$$v(\vec{r}) = \frac{1}{2} \int w(\vec{r}, \vec{r}') d^3\vec{r}' \quad (\text{A-14})$$

It is defined such that its integral over all space is the total interaction energy W .

References

1. R. G. Seyler and C. H. Blanchard, Phys. Rev. 124 (1961) 227; 131 (1963) 355
2. W. D. Myers and W. J. Swiatecki, Ann. Phys. 55 (1969) 395
3. J. Blocki, J. Randrup, W. J. Swiatecki, and C. F. Tsang, Lawrence Berkeley Laboratory Preprint LBL-3603, to be published
4. J. Randrup, Lawrence Berkeley Laboratory Preprint LBL-4308, submitted to Phys. Lett. B
5. H. Gräf, private communication (1974), to be published
6. G. Süssmann, Lawrence Berkeley Laboratory Report, LBL-1615 (1973)
7. W. D. Myers, Nucl. Phys. A204 (1973) 465
8. M. A. Thorpe and D. J. Thouless, Nucl. Phys. A156 (1970) 225
9. W. J. Swiatecki, Proc. Phys. Soc. A68 (1955) 353

TABLE 1. Results for the surface diffuseness t_{10-90} and the surface energy a_s , for various values of the parameter η . The upper results are obtained in the modified Thomas-Fermi approximation while the lower results are obtained in the Hartree approximation.

η	-1.0	-0.5	0.0	0.5
t_{10-90} (fm)	3.58 3.70	2.88 2.95	1.99 2.22	0.53 1.71
a_s (MeV)	29.25 30.34	24.48 25.85	18.56 20.55	9.77 13.75

Figure Captions

- Fig. 1. Surface diffuseness. As a function of the parameter η is plotted the surface diffuseness of the equilibrium matter density distribution, obtained with the modified Thomas-Fermi approximation. As well the 10-90% diffuseness t_{10-90} as the second surface moment b are displayed. The crosses indicate results obtained in the Hartree approximation. The values corresponding to an infinitely high potential wall are also indicated.
- Fig. 2. Surface energy. As function of the parameter η is plotted the surface energy coefficient a_s for the equilibrium solution obtained with the modified Thomas-Fermi approximation. The crosses indicate results obtained in the Hartree approximation.
- Fig. 3. Surface energy versus surface diffuseness. The curve labeled "equilibria" joins the locations of the Thomas-Fermi equilibrium solutions obtained for a series of values of the parameter η . The abscissa is the 10-90% matter diffuseness t_{10-90} (Fig. 1) and the ordinate is the surface energy coefficient a_s (Fig. 2). The curve labeled " a_s^0 " is the contribution to the surface energy originating from the η -independent part of the Hamiltonian; it is to a very good approximation identical to what would result from simply stretching or compressing the equilibrium solution corresponding to $\eta = 0$. The curve labeled " δa_s " is the contribution to the surface energy due to the η -dependent term (with the η divided away). The total surface energy $a_s = a_s^0 + \eta \delta a_s$ is plotted as function of the diffuseness for some values

of η (dashed curves). The crosses indicate the self-consistent Hartree solutions calculated for four selected values of η .

Fig. 4. Matter density distribution (in units of the bulk value) for four selected values of the parameter η . The dashed curves are the results obtained with the modified Thomas-Fermi approximation while the Hartree results are shown by the full curves.

Fig. 5. Matter density distributions for $\eta = 0$. The Thomas-Fermi density is labeled "TF". The undulating curve is the density obtained in the Hartree approximation. The dashed curve is the density that would result for an infinite wall (positioned so that the undulations are in phase inside the system).

Fig. 6. Kinetic distributions (in units of the bulk value) for $\eta = 0$. The dashed curve is the Thomas-Fermi kinetic density γ_{TF} while the full curve is the Hartree kinetic density denoted $\gamma (= \frac{1}{2} (\kappa + \tau))$. The lower curve is the distribution $\delta (= \frac{1}{2} (\kappa - \tau))$.

Fig. 7. Surface energy density distribution. The dashed curve is the Thomas-Fermi result and the full curve the Hartree result.

Fig. 8. Decomposition of the surface energy density into the kinetic and interaction parts. Dashed curve: Thomas-Fermi, full curve: Hartree.

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Fig. 1

Fig. 2

Fig. 3

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Fig. 4

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Fig. 5

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Fig. 6

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Fig. 7

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Fig. 8

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