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A MODIFIED THOMAS-FERMI TREATMENT OF NUCLEI

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Abstract

An improved nuclear Thomas-Fermi theory is studied in which, rather than adding density-gradient corrections to the standard expression for the kinetic-energy density (proportional to $\rho^{5/3}$, where ρ is the density) one simply modifies this $\rho^{5/3}$ function to reflect the fact that the kinetic energy density becomes negative for small values of ρ when, in a typical nuclear problem, one is dealing with the outer fringes of the surface region. The net result of this study is simply stated: in order to find the density associated with a given nuclear potential, one exponentiates this potential instead of raising its depth with respect to the chemical potential to the three-halves power, as in the standard treatment. An improved description of the nuclear surface profile is obtained, including the quantal halo in the classically forbidden region. But since density derivatives are not involved, there is no need to solve a partial differential equation in order to find the density.

1. Introduction

Statistical theories of atomic or nuclear ground-state density distributions $\rho(\vec{r})$ are based on making the system's energy stationary with respect to particle-preserving variations $\delta\rho(\vec{r})$. The energy is usually written as an integral over all space of the sum of suitable kinetic and interaction energy densities, say t and w, respectively. In general, t and w may be *functionals* of the density $\rho(\vec{r})$. The variation of the total energy E can then be written as

$$\delta E = \int d^3r \left(\frac{\delta t}{\delta\rho} + V\right) \delta\rho \,, \tag{1}$$

where $\delta t/\delta\rho$ is the functional variation of t. The quantity V, equal to the functional variation $\delta w/\delta\rho$, represents the *potential* which, when multiplied by $\delta\rho$ and integrated over all space, gives the change in the interaction energy.

In order for δE to vanish for particle-preserving variations, for which $\int d^3r\, \delta\rho = 0$, it is sufficient that the integrand in Eq. (1) should be a constant, i.e.

$$\frac{\delta t}{\delta\rho} + V = \text{constant} = L, \text{ say} \quad . \tag{2}$$

Here L is the Lagrange multiplier in the Euler eq. (2). For a *non*-particle-preserving variation $\delta\rho$, eq. (1) would give

$$\delta E = L \int d^3r\, \rho = L\delta N,$$

where δN is the change in the particle number. Thus L is the chemical potential, dE/dN, or, in the nuclear context, L is minus the separation energy S.

In the standard Thomas-Fermi approximation, the kinetic energy density t is not a functional of $\rho(\vec{r})$ but a simple function of the local density ρ, which may be written as

$$t = \tfrac{3}{5} C\rho^{5/3}, \tag{3}$$

where C is a known constant. (For standard nuclear matter $C = (3h^3/16\pi)^{2/3}/2m$, where h is Planck's constant and m the nucleon mass.) The Euler equation becomes now

$$C\rho^{2/3} + V = L. \tag{4}$$

In cases where an external (non-self-consistent) potential $V(\vec{r})$ is given (or when, in a self-consistent theory, $V(\vec{r})$ is available at an intermediate step of an iterative solution of eq. (4), as in Ref. 1), the density is trivially found to be given by

$$\rho(\vec{r}) = \left(\frac{L - V(\vec{r})}{C}\right)^{3/2}. \tag{5}$$

In a class of theories seeking to improve the standard Thomas-Fermi method (whose principal failing is its inability to describe the density in the classically forbidden region, where L – V is negative) t is made a functional of ρ or, more simply, a function of ρ and of its local spacial derivatives. These generalized theories are frequently based on power expansions in the derivatives of ρ (or of V), formally valid when these derivatives are small, but often yielding accurate results even when this formal requirement does not appear to be satisfied (Ref. 2,3).

In the present paper we shall examine a different type of modification of the Thomas-Fermi method, one in which $t(\rho)$ is still a simple local function of ρ only, but a function different from $\frac{3}{5} C\rho^{5/3}$. One reason for exploring this type of theory is that the resulting Euler equation remains a straightforward relation between ρ and V, rather than a *differential equation* involving the derivatives of ρ. This is a simplification of enormous practical significance in the treatment of, for example, deformed nuclei, where one would otherwise have to solve a *partial*

differential equation in three dimensions. (In fitting by least squares the parameters of a Thomas-Fermi theory to the binding energies of hundreds of nuclei, it might be necessary to solve such partial differential equations many thousands of times.)

2. The Modified Thomas-Fermi Method

What modification of the standard Thomas-Fermi method is called for in the case of nuclei, consisting typically of a bulk region and a surface region? In the bulk the Thomas-Fermi method may be adequate, so the new function may well continue to be $\frac{3}{5}C\rho^{5/3}$ when ρ is not too different from its bulk value. At the other extreme, when ρ is close to zero, one is typically in the classically forbidden region in the outer fringe of the surface. In this region the quantal tails of the particles' wave functions have negative kinetic energies, so the modified kinetic energy density should turn negative for small ρ. Moreover, in the *extreme* fringe of the surface, the wave functions with the longest exponential tails will predominate. These are the least bound wave functions, whose tails are governed by the separation energy S. Hence the kinetic energy per particle in the extreme fringe will tend to minus S, and the energy density will tend to $-S\rho$ as ρ tends to zero. The question then becomes how to interpolate between $\frac{3}{5}C\rho^{5/3}$ and $-S\rho$ in order to obtain a useful local approximation to the kinetic energy density. We shall attempt to answer this question by examining the exact density in a typical surface problem, where a gas of non-interacting nucleons with Fermi energy T_o is bounded by an infinite diffuse plane surface described by a Woods-Saxon potential V(x) of depth U_o and diffuseness a, viz.:

$$V(x) = -\frac{U_o}{1 + e^{x/a}} \quad . \tag{6}$$

Imagine that the exact density $\rho(x)$ has been determined for this problem. Since the Euler equation now reads

$$\frac{dt}{d\rho} = -V(x) - S \quad , \tag{7}$$

and since the relation between ρ and x (or x and ρ) is assumed to have been calculated, eq. (7) may be regarded as an equation for $dt/d\rho$ expressed as a function of ρ. Simple integration of this expression will then give that purely local energy density $t(\rho)$ which, by construction, is guaranteed to reproduce the exact density $\rho(x)$ when inserted in the Euler equation. Let us examine what such a function $t(\rho)$ actually looks like.

The circled points in Fig. 1 show the exact density $\rho(x)$ in units of its bulk value ρ_o, for a Woods-Saxon potential with $U_o = 56$ MeV and $a = 0.6$ fm, filled with standard nuclear matter up to a Fermi energy $T_o = 37.7602$ MeV, corresponding to a Fermi wave number $k_o = 1.35\ \mathrm{fm}^{-1}$ (i.e., to a nuclear matter radius constant $r_o = (9\pi/8)^{1/3}/k_o = 1.1283$ fm). The above density was calculated numerically by Durand et al., Ref. 3. The separation energy S is 56–37.7602 = 18.2398 MeV in this case. The standard Thomas-Fermi approximation is also plotted in Fig. 1. The exact density differs from it in three respects: a density tail extending into the classically forbidden region, an approximately compensating density deficiency in the intermediate region of the surface profile (extending to about $\rho/\rho_o = 0.87$), followed by relatively small Friedel oscillations for $\rho/\rho_o \gtrsim 0.87$.

Figure 2 shows $dt/d\rho$ obtained by inserting the exact relation between x and ρ into eq. (7). The plot uses dimensionless quantities defined by $\chi \equiv \rho/\rho_o$ and $\tau \equiv t/T_o\rho_o$. In these units the Thomas-Fermi energy density is $\tau_{TF} = \frac{3}{5}\chi^{5/3}$, and its derivative is simply $\chi^{2/3}$, also plotted in Fig. 2. The dimensionless Euler equation may now be written as

$$\frac{d\tau}{d\chi} = \frac{-V-S}{T_o} = 1 - u \quad , \tag{8}$$

where the dimensionless quantity u(x) is the Woods-Saxon potential, in units of T_o, measured from the bottom up, i.e., $u = 0$ for $x \to -\infty$, and $u = 1 + \sigma$ for $x \to \infty$, where $\sigma = S/T_o$.

The circles in Fig. 2, considered as displaying $d\tau/d\chi$ as a function of χ, define the dimensionless kinetic energy density derivative that reproduces the exact density in Fig. 1. Note that turning Fig. 2 on its side and regarding it as a plot of χ versus u (u and $d\tau/d\chi$ being related by eq. (8)), corresponds simply to re-plotting the density profile from Fig. 1, except that χ is now displayed not as a function of x but as a function of the potential u at x. In this plot the classically forbidden tail is again in evidence for $u > 1$, the compensating density deficiency with respect to the Thomas-Fermi curve appears for $u > 1 - (0.87)^{2/3} \approx 0.09$, and the Friedel oscillations are now squashed into a rather insignificant slot of u-values below 0.09.

The function represented by the circled points may be approximated as follows:

$$\chi = (1-u)^{3/2} \quad , \quad \text{for} \quad 1 > \chi > \chi_1 \quad , \tag{9}$$

$$\chi = C_1 e^{-u/c} - C_2 \ , \quad \text{for} \quad 0 < \chi < \chi_1 \ , \tag{10}$$

where $\chi_1 = 0.87$ and C_1, C_2 and c are constants. Solving eq. (10) for u and inserting in eq. (8) we find

$$\frac{d\tau}{d\chi} = 1 + c \ln \frac{\chi + C_2}{C_1} \ . \tag{11}$$

Integrating, we obtain the following explicit representation of the kinetic energy density $\tau(\chi)$:

$$\tau = \chi + c\left[(C_2 + \chi) \ln \frac{\chi + C_2}{C_1} - \chi - C_2 \ln \frac{C_2}{C_1}\right] . \tag{12}$$

The values of the three constants C_1, C_2 and c are determined uniquely by the following three requirements of continuity, smoothness and asymptotic behaviour of $\tau(\chi)$:

$$\tau(\chi_1) = \tau_{TF}(\chi_1) = \tfrac{3}{5}\chi_1^{5/3} \tag{13}$$

$$\tau'(\chi_1) = \tau'_{TF}(\chi_1) = \chi_1^{2/3} \tag{14}$$

$$\tau(\chi) \to -\sigma\chi \quad \text{for} \quad \chi \to 0 \ . \tag{15}$$

The last equation is the dimensionless form of the requirement $t \to -S\rho$, discussed earlier.

Note that eq. (13), which demands that the integrals from 0 to χ_1 of $\tau'(\chi)$ and $\tau'_{TF}(\chi)$ in Fig. 2 be equal, corresponds to the requirement that the density excess in the tail and the subsequent density deficiency in the intermediate regime of the surface profile (when this profile is plotted against the potential rather than the distance) should be *exactly* equal. In other words, the areas of the two major excursions of $\tau'(\chi)$ around $\tau'_{TF}(\chi)$ in Fig. 2 should be equal. This 'theorem' (based on the assumption of a purely local function $t(\rho)$ which becomes equal to $t_{TF}(\rho)$ near the bulk density) appears to be quite well satisfied by the exact density, represented by the circled points in Fig. 2.

It is readily verified that eqs. (13–15) result in the following algorithm for calculating C_1, C_2 and c. First solve numerically for the quantity Z in the equation

$$e^{1/Z} - 1 - (Z - Z_1)^{-1} = 0 \ , \tag{16}$$

where

$$Z_1 = \tfrac{2}{5}\chi_1^{2/3} \Big/ (\chi_1^{2/3} + \sigma) \quad . \tag{17}$$

Then the values of c and C_2 are given by

$$c = (\chi_1^{2/3} + \sigma)\, Z \tag{18}$$

$$C_2 = \chi_1 (Z - Z_1) \quad , \tag{19}$$

and the value of C_1 follows from

$$C_1 = C_2\, e^{(1+\sigma)/c} \quad . \tag{20}$$

With $\chi_1 = 0.87$ and $\sigma = 18.2398/37.7602 = 0.483043$, we find $c = 0.414508$, $C_1 = 1.116103$ and $C_2 = 0.031179$. In Figs. 1 and 2 the resulting approximation to the circled points is indicated. Figure 3 shows the corresponding function $\tau(\chi)$, together with the conventional Thomas-Fermi approximation. Thus, by a relatively small modification of the Thomas-Fermi energy density, one that makes τ turn slightly negative before its approach to zero, one obtains a *local* energy density function that will reproduce closely the exact density profile. In particular, the density tail in the classically forbidden region is reproduced approximately.

But is this scheme, represented by eqs. (9-20), useful in situations other than the one that inspired its construction? In particular, will it work also when the separation energy is reduced from 18.2398 MeV toward zero?

Figures 4(a), (b) and (c) show the results of applying the above equations to 3 additional cases (kindly supplied by the Authors of ref. 3), with T_o kept fixed, and U_o equal to 54, 46 and 38 MeV, so that S = 16.2398, 8.2398 and 0.2398 MeV, respectively. It is clear that in all cases a comparable improvement over the standard Thomas-Fermi method is obtained. Note that no parameters have been re-adjusted. The only parameter in the whole scheme is χ_1, equal to 0.87, representing the relative density above which the standard Thomas-Fermi method is deemed adequate.

The net results of the rather elementary modification of the Thomas-Fermi "three-halves power" rule, i.e., $\chi = (1 - u)^{3/2}$, to the "exponential" rule $\chi = C_1 e^{-u/c} - C_2$ for $\chi < \chi_1$, is that for a typical nuclear (surface) problem one

continues to have available an explicit expression for the density $\rho(\vec{r})$ in terms of the potential $V(\vec{r})$, one that for some purposes could be used in place of the exact solution.

3. An Application

The effect of the present modification of the Thomas-Fermi method is to shift matter from the classically allowed region of the surface, where the kinetic energy is positive, to the classically forbidden region, where it is negative. The result is to lower the kinetic energy and thus to make more negative the already negative kinetic-energy contribution to the nuclear surface energy. (The kinetic energy contributes negatively because, for a typical nuclear potential, particles entering the surface are slowed down and their kinetic energies are reduced.) Other things being equal, this would show up as a considerable lowering of the nuclear surface energy. But in phenomenological theories of nuclear binding energies, in which adjustable parameters are used, the surface energy is, in effect, one of the quantities to which the parameters are adjusted. Thus, when used in this sense, both the standard and the modified thomas-Fermi theories would, by construction, reproduce the surface energy. However, even after such adjustment of parameters, the two theories may be expected to make rather different predictions about the nuclear *curvature energy* (the correction to the surface energy caused by the curvature of the surface). This is because the curvature energy is sensitive to finer details of the surface profile, which is significantly altered in the modified Thomas-Fermi theory.

The curvature energy coefficient a_3 may be defined as the coefficient of $A^{1/3}$ in the binding energy of uncharged spherical nuclei with mass number A, written as an expansion in $A^{-1/3}$:

$$BE = -a_1 A + a_2 A^{2/3} + a_3 A^{1/3} + \dots \ . \tag{21}$$

(The binding energy is assumed to have been corrected for the effect of compressibility, which is also of order $A^{1/3}$, Ref. 4.)

In the theory of the curvature energy, as described in Ref. 4 and summarized in the Appendix, a_3 consists of two parts, which may be called 'geometrical' and 'non-local':

$$a_3 = a_{3G} + a_{3N} \ . \tag{22}$$

The former arises from the geometrical fact that for a convexly curved surface (with a given density profile) the relative number of surface particles towards the bulk is decreased in relation to the number of particles in the tail. (For a spherically symmetric system this is due to the r^2 weighting of volume elements.) The non-local part a_{3N} has to do with the fact that when the energy density at a point in the surface is a non-local function of the density, the conditions at that point are modified when the surface is curved. For example, a particle on the surface of a sharp, curved density distribution has fewer neighbours within a given interaction range than when the surface is flat. The Thomas-Fermi model of Ref. 4 illustrates these features. Thus a_{3G} was found to be –19.42 MeV, a_{3N} was +28.76 MeV, giving a resulting curvature energy coefficient $a_3 = 9.34$ MeV. This is a value typical of theoretical estimates of a_3, which appears to have led to a 'curvature energy puzzle,' because empirical evidence seems to suggest a smaller value, consistent with $a_3 \approx 0$ (Ref. 5).

When the energy density η consists of a kinetic energy density t and an interaction energy density w, the geometrical and non-local parts consist each of two contributions, associated with t and w, viz., $a_{3G} = a_{3G}(t) + a_{3G}(w)$, $a_{3N} = a_{3N}(t) + a_{3N}(w)$. In models such as the one studied in the present paper, where the kinetic energy density is assumed to be local, the non-local term $a_{3N}(t)$ is zero, and a_3 consists of three parts:

$$a_3 = a_{3G}(t) + a_{3G}(w) + a_{3N}(w) \,. \tag{23}$$

We shall now calculate the first of these terms in the standard and modified theories, for the system corresponding to Fig. 1, in order to estimate the possible effect on a_3 arising from the presence of a quantal halo in the classically forbidden region of the surface. The formula for $a_{3G}(t)$, as derived in the Appendix, is

$$a_{3G}(t) = \tfrac{18}{5} T_o \int_{-\infty}^{\infty} dv\, v\, (\theta - \chi) \,, \tag{24}$$

where v is the normal distance from the effective sharp surface of the density profile in units of the radius constant r_o of the bulk matter (equal to 1.1283 fm in the present case) and $\theta = t/t_o$, where $t_o = \frac{3}{5} T_o \rho_o$. The function $\theta - \chi$ is plotted in the lower part of Fig. 1. It is immediately obvious that the first moment of this function appearing in Eq. (24) (taken with respect to the effective sharp surface, which is located at $x_o = -0.79_5$ fm in the standard theory and

at $x_o = -0.80_6$ fm in the modified one) will be considerably smaller in the modified theory because of the negative tail in $\theta - \chi$. Numerical integration yields, in fact:

$$a_{3G}(t) = 5.9 \text{ MeV} \qquad \text{(Thomas-Fermi)}$$

$$a_{3G}(t) = -11.0 \text{ MeV} \qquad \text{(Modified Thomas-Fermi)} \quad .$$

The very considerable lowering of $a_{3G}(t)$ by the quantal halo makes this physical effect a candidate for solving the curvature energy puzzle mentioned earlier. To reach a decision on this point it will be necessary to carry out a self-consistent calculation in which the effect of the quantal tail on the terms $a_{3G}(w)$ and $a_{3N}(w)$ is evaluated, and the surface energy in the modified theory is refitted to the empirical value. Work on this problem is in progress.

4. Discussion

The present attempt to improve the standard Thomas-Fermi method differs from most previous ones by not relying on a power expansion in the gradient of the density, or of the potential or, equivalently, on a formal expansion in Planck's constant $\hbar$. (The smallness parameter in question is proportional to the ratio ε of an average particle's wavelength to the diffuseness of the nuclear surface.) There are both good and bad aspects of our approach. On the one hand it avoids the reservations one might have concerning the smallness of ε in actual situations of interest, and the possible importance of non-analytic terms of the type $e^{-1/\varepsilon}$, relevant in the quantal tail but not amenable to a power expansion. (Numerical studies seem to indicate that such reservations are much less serious than one might have thought, Ref. 3.) In our method one examines a surface with a realistic ratio of wavelength to diffuseness, and tries to embody the physics of the situation (including the quantal halo) in a simple equation for the kinetic energy density. The drawback of this method is precisely that it is not a systematic approximation scheme, whose accuracy is well understood and is controlled by a well-defined expansion parameter. In novel situations the method might begin to break down in some unexpected way. A simple example of where it does break down is the case of a *uniform*, infinite Fermi gas with low density. In that case, no matter how low the density, the actual kinetic energy density never becomes negative (and the *unmodified* Thomas-Fermi theory is actually exact). But, in the nuclear context, uniform low density matter is not usually of interest, certainly not as a stable ground state distribution. In most practical situations of interest, low densities are only found in the fringes of

nuclear surfaces, and there the kinetic energy density *is* negative. One could argue that in such cases it is sensible to put this physical feature of the kinetic energy density explicitly into the formalism, rather than hoping that gradient corrections will do the job. However that may be, a very attractive feature of the present method, and one reason for examining it further, is its relative simplicity, avoiding as it does the need to solve partial differential equations. But how useful the method will turn out to be in practice still remains to be seen.

Appendix

Here we summarize the theory of the surface and curvature energies in the special case of spherically symmetric systems. (The general case is discussed in Refs. 4, 6.)

The energy of a thin-skinned (leptodermous) system, written as

$$E = \int_0^\infty dr\, 4\pi r^2 \eta$$

is identically equal to

$$E = e_o A + 4\pi \int_0^\infty dr\, r^2 (\eta - e_o \rho) , \tag{A1}$$

where $\rho(r)$ is the density, $\eta(r)$ the energy density (both falling off from ρ_o, η_o in the bulk to zero in a thin surface region), $A = \int_0^\infty dr\, 4\pi r^2 \rho$ is the total number of particles and e_o is the energy per particle in the bulk, equal to η_o/ρ_o. The first term in eq. (A1) is the volume energy and the second is a surface-layer correction. This correction is associated with the surface because, for a leptodermous system, the integrand $[\eta - (\eta_o/\rho_o)\rho]$ is obviously confined to a thin surface layer. Because of this localization it is convenient to change the variable of integration to n, where $r = R + n$, and R is the effective sharp radius defined by $A = (4\pi/3)R^3\rho_o$. The surface-layer correction becomes

$$E_{SL} = 4\pi \int_0^\infty dn (R + n)^2 F(n) , \tag{A2}$$

where $F(n) = \eta - e_o\rho$ is the 'surface-energy function.' It is a function of position, localized in the surface. Denoting its limit for a plane surface by $F_o(n)$ and expanding to first order in the curvature κ, where $\kappa = 2/R$ for a sphere of radius R, we have

$$F(n) = F_o(n) + F_o'(n)\,(2/R) + \dots , \tag{A3}$$

where $F_o'(n)$ is the derivative of F(n) with respect to curvature, evaluated for zero curvature, i.e., for plane geometry. Inserting in Eq. (A2) we find

$$E_{SL} = 4\pi \int_{-\infty}^{\infty} dn(R^2 + 2Rn + \cdots)\,(F_o + \frac{2}{R} F_o' + \cdots)$$

$$= 4\pi R^2 \int_{-\infty}^{\infty} dnF_o(n) + 8\pi R \int_{-\infty}^{\infty} dnnF_o(n) + 8\pi R \int_{-\infty}^{\infty} dnF_o'(n) \quad . \tag{A4}$$

The lower limit of integration has been taken as $-\infty$ since $F_o(n)$ and $F_o'(n)$ are assumed to be localized in the surface. Writing $R = r_o A^{1/3}$, we find

$$E_{SL} = A^{2/3} \cdot 4\pi r_o^2 \int_{-\infty}^{\infty} dnF_o + A^{1/3} \cdot 8\pi r_o \int_{-\infty}^{\infty} dnnF_o + A^{1/3} \cdot 8\pi r_o \int_{-\infty}^{\infty} dnF_o' \quad . \tag{A5}$$

The first term is the surface energy $a_2 A^{2/3}$, the second is the geometrical part of the curvature energy, $a_{3G} A^{1/3}$, and the last the non-local part $a_{3N} A^{1/3}$. We now focus attention on the contribution to a_{3G} coming from the kinetic energy density t. Since $\eta = t + w$, and $e_o = \eta_o/\rho_o = (t_o + w_o)/\rho_o$, we have (droping the subscript zero on F(n) that denotes plane geometry)

$$F(n) = t + w - (t_o + w_o)\rho/\rho_o = \left(t - \frac{t_o}{\rho_o}\rho\right) + \left(w - \frac{w_o}{\rho_o}\rho\right) ,$$

so that the kinetic energy part of a_{3G} becomes

$$a_{3G}(t) = 8\pi r_o \int_{-\infty}^{\infty} dnn\left(t - \frac{t_o\rho}{\rho_o}\right) = 8\pi r_o t_o \int_{-\infty}^{\infty} dn\, n\left(\frac{t}{t_o} - \frac{\rho}{\rho_o}\right) .$$

Since t_o, the kinetic energy density in the bulk, may be written as

$$\text{(kinetic energy per particle)} \times \text{(density)} = \left(\frac{3}{5} T_o\right)\left(\frac{4}{3}\pi r_o^3\right)^{-1} ,$$

we find

$$a_{3G}(t) = \frac{18}{5} T_o \int_{-\infty}^{\infty} dv v (\theta - \chi) , \tag{A7}$$

where $v = n/r_o$, $\theta = t/t_o$ and $\chi = \rho/\rho_o$. This is the formula used in the text to calculate $a_{3G}(t)$.

Note also that the kinetic-energy contribution to the surface energy coefficient a_2 is

$$a_2(t) = 4\pi r_o^2 t_o \int_{-\infty}^{\infty} dn \left(\frac{t}{t_o} - \frac{\rho}{\rho_o}\right) = \frac{9}{5} T_o \int_{-\infty}^{\infty} dv(\theta - \chi) . \tag{A8}$$

Its value in the example illustrated in Fig. 1 is –18.15 MeV for the standard theory and –26.89 MeV for the modified one.

Acknowledgements

The present study is the outcome of an analysis of the accurate numerical solutions of the semi-infinite Woods-Saxon surface problem described in Ref. 3. I would like to express my indebtedness to the Authors of that work, and to M. Durand for providing me with the exact densities on which Figs. 4a,b,c are based. Discussions with W.D. Myers and discussions and correspondence with P. Schuck were also very helpful.

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Figure Captions

Fig. 1. The upper part shows the exact relative density ρ/ρ_o (circles) and the standard and modified Thomas-Fermi approximations in the case of a Fermi gas bounded by a semi-infinite, plane Woods-Saxon potential, displayed in units of the Fermi energy T_o (right scale, labeled u). The locations of the three effective sharp surfaces are almost indistinguishable and are indicated by x_o. The lower part shows the kinetic energy part of the surface energy functions, $\theta-\chi$, in the standard and modified Thomas-Fermi approximations. The figure corresponds to a separation energy S = 18.2398 MeV.

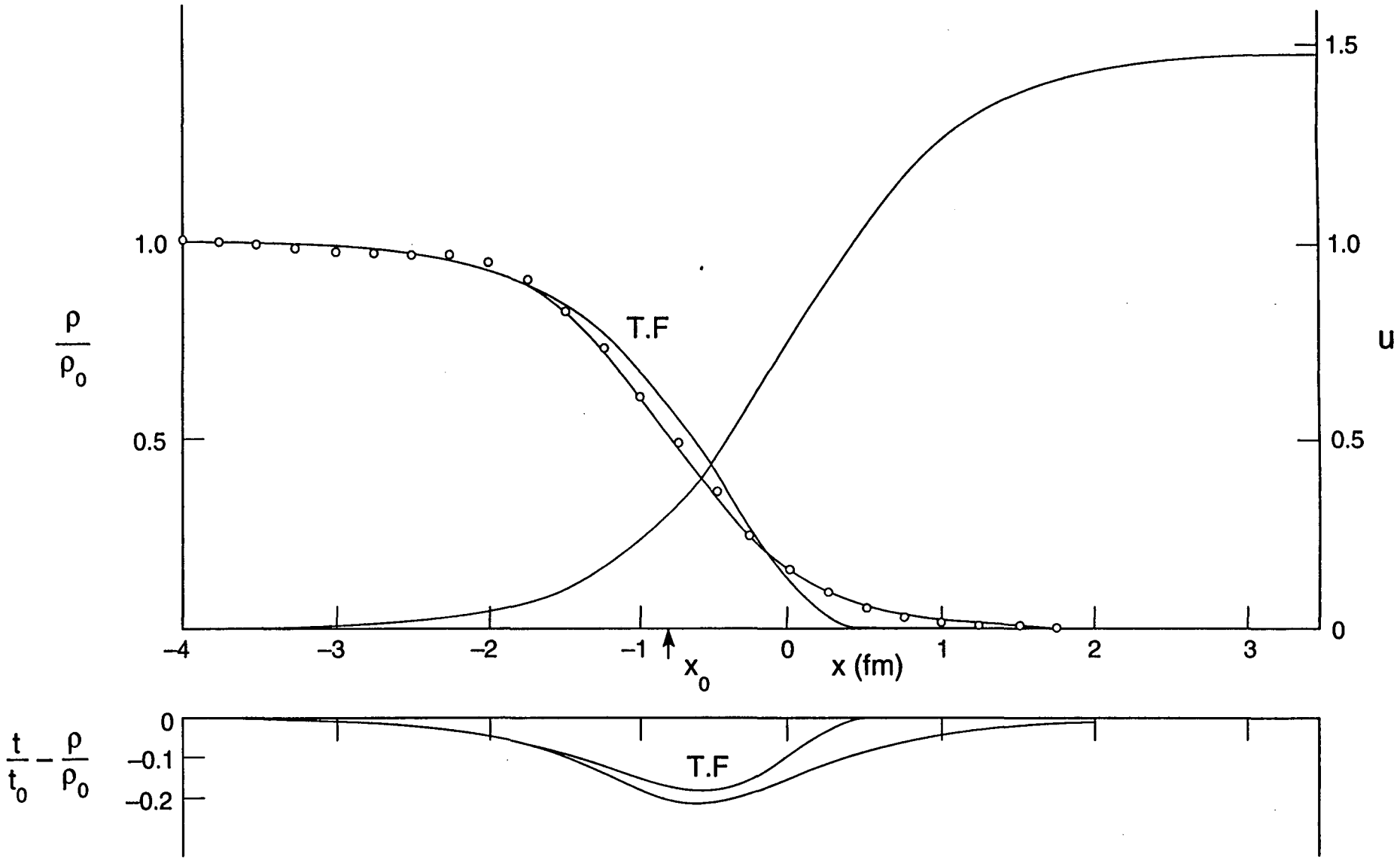
Fig. 2. The derivative of the relative kinetic energy density, $\tau'(\chi)$, is plotted against the relative density χ. The Thomas-Fermi curve is given by $\chi^{2/3}$. The circles define that kinetic energy density derivative which, when inserted in the Euler equation, would reproduce the exact density in Fig. 1. The approximation to the circled points underlying the modified Thomas-Fermi theory is also shown. Using the Euler equation in the form $\tau' = 1 - u$, Fig. 2, when turned on its side, may be regarded as equivalent to a plot of the density profile in Fig. 1, but displayed as a function of the potential u at x rather than of the position x.

Fig. 3. The Thomas-Fermi relative energy density $\frac{3}{5}\chi^{5/3}$ and the modified function are shown. The latter is given by eq. (12) in the text. It turns negative at low densities and approaches zero with a negative slope determined by σ, equal to the separation energy S in units of T_o.

Fig. 4(a). Same as the upper part of Fig. 1, but for a separation energy S = 16.2398 MeV.

Fig. 4(b). Same as Fig. 4(a), but for a separation energy S = 8.2398 MeV.

Fig. 4(c). Same as Fig. 4(a), but for a separation energy S = 0.2398 MeV.



XBL 9110-6818

Figure 1

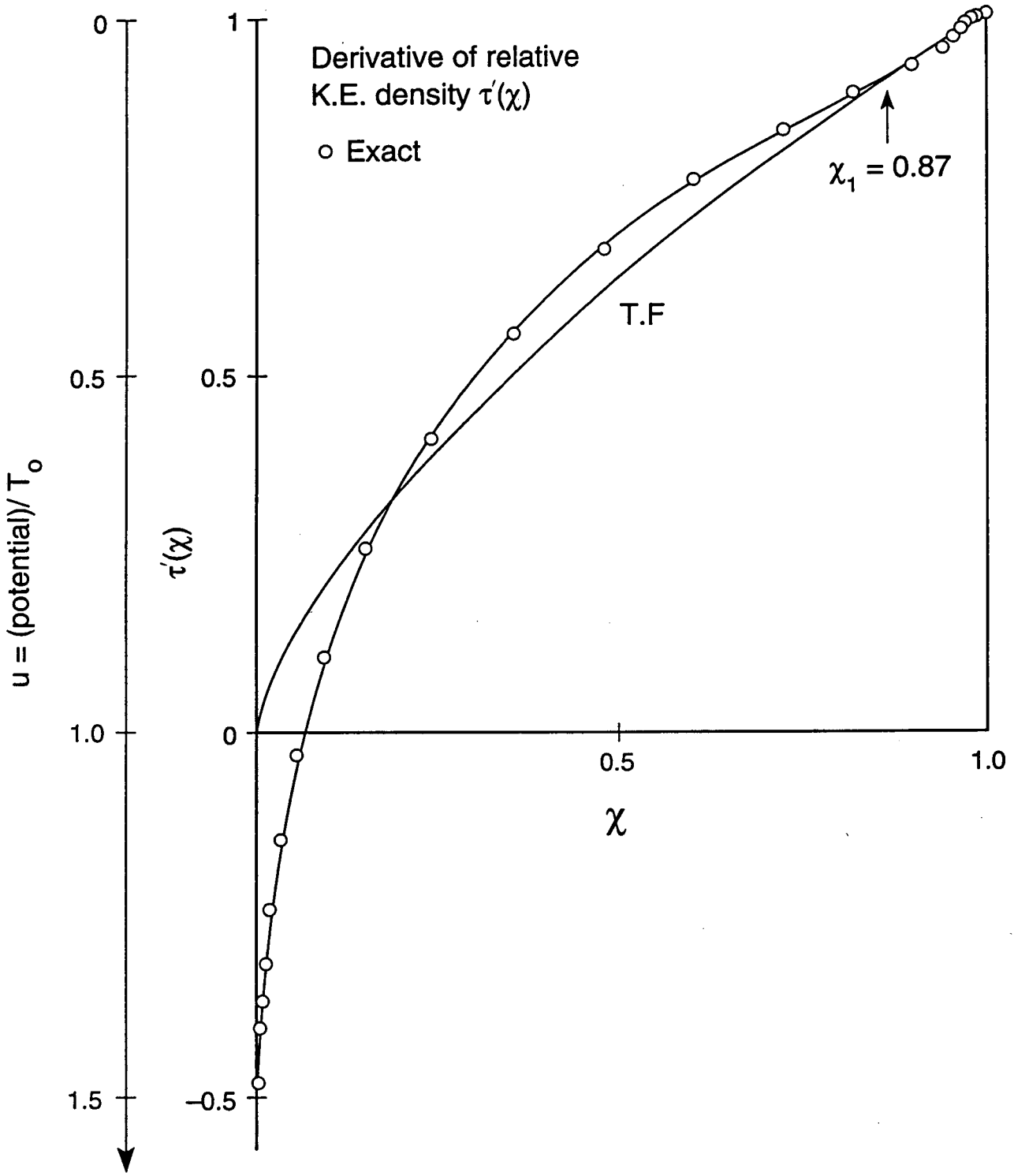


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Figure 2

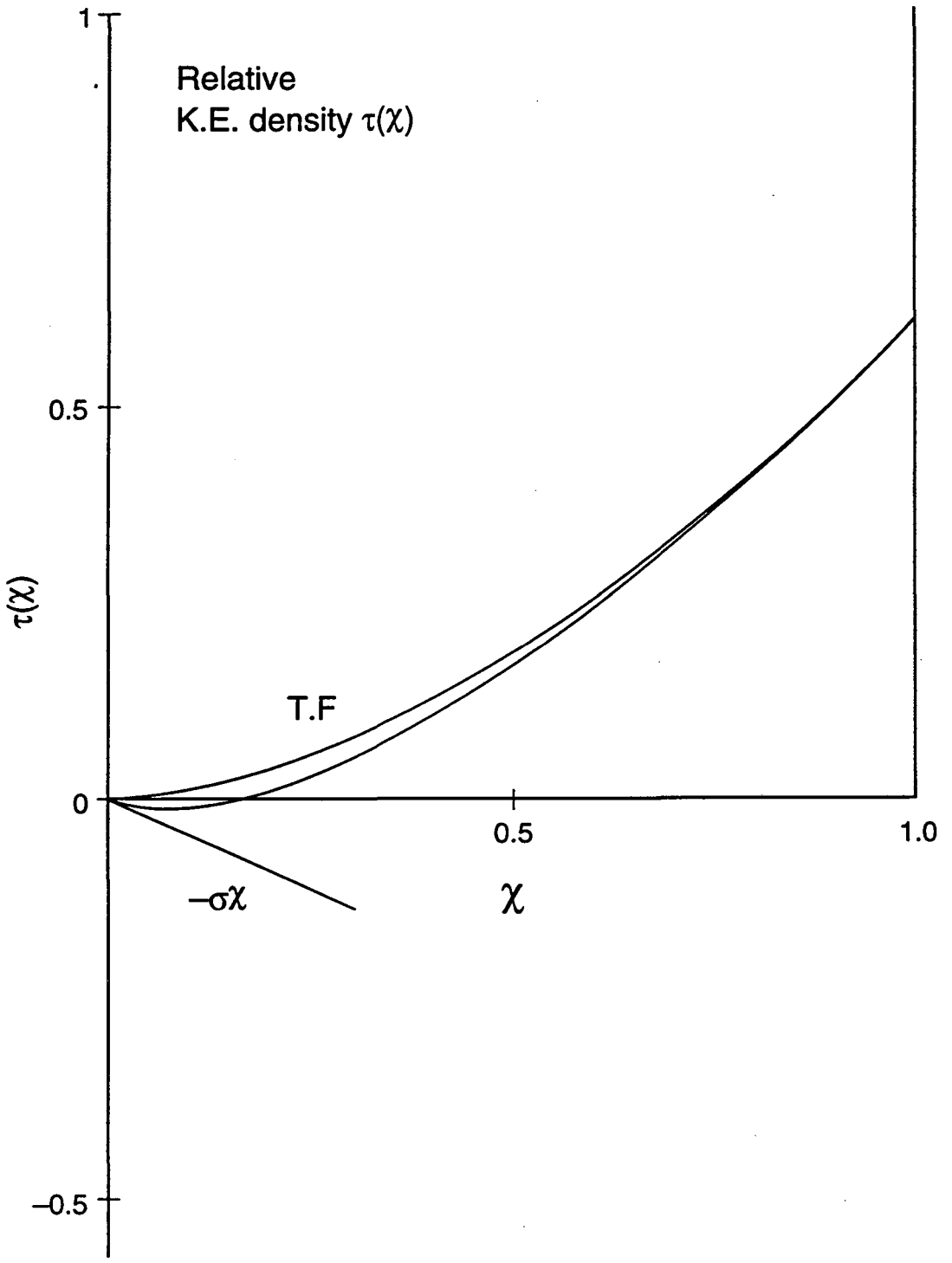

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Figure 3

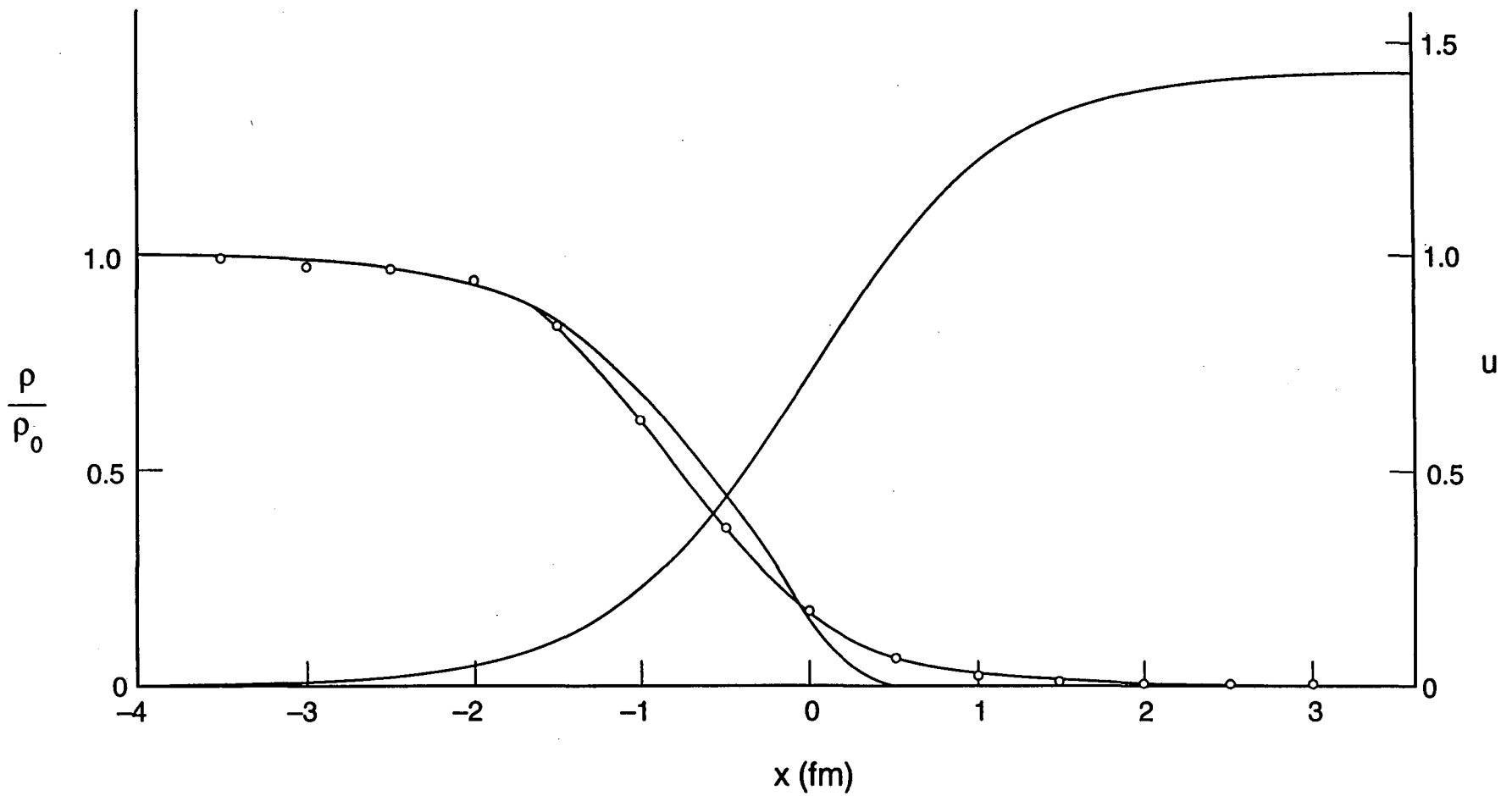

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Figure 4(a)

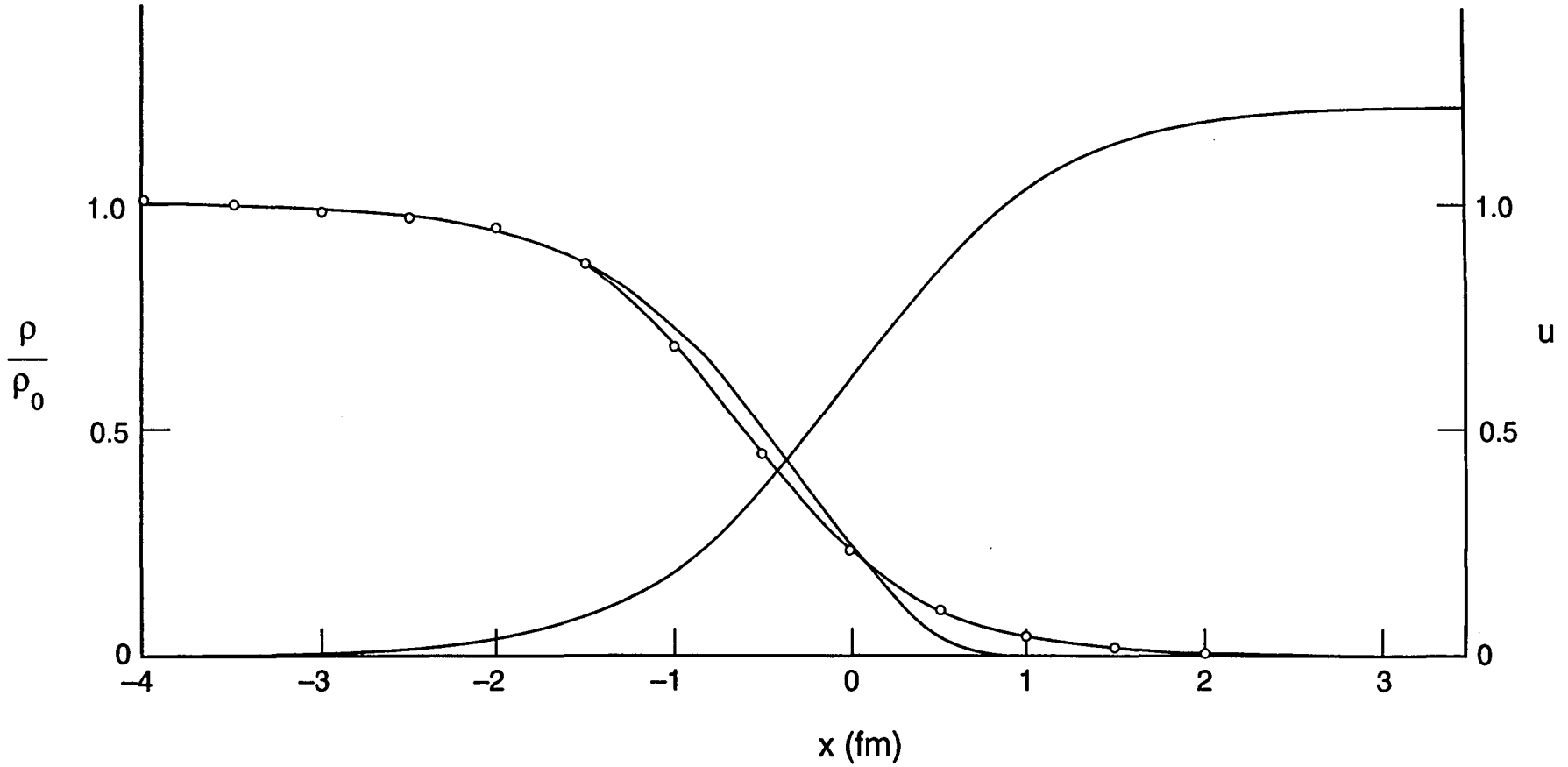

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Figure 4(b)

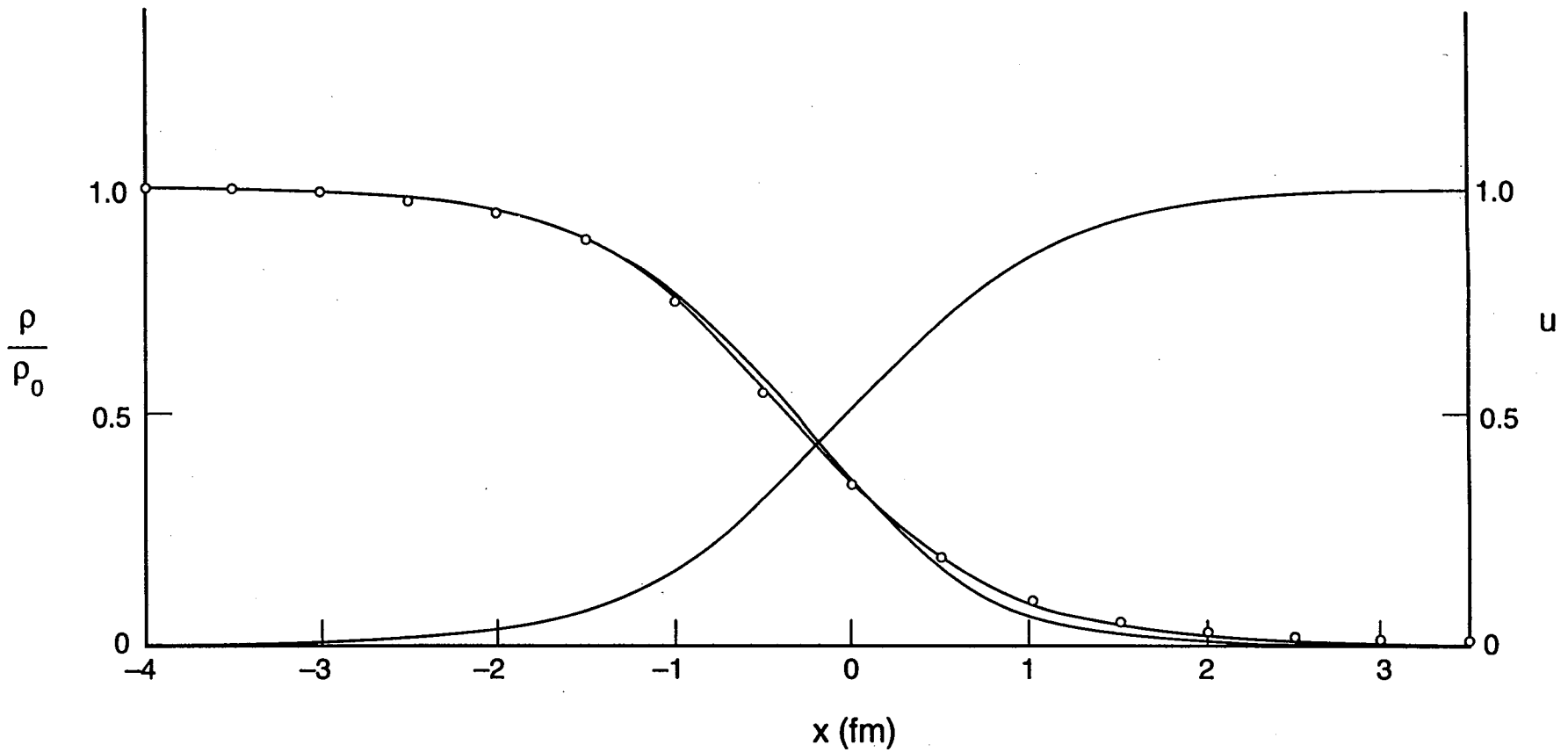

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Figure 4(c)

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