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An Improved Thomas-Fermi Treatment of Nuclei

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1. INTRODUCTION

I want to tell you about an improved Thomas-Fermi method for calculating shell-averaged nuclear properties, such as density distributions, binding energies, etc. (Ref. 1). A shell-averaged statistical theory is useful as the macroscopic component of microscopic-macroscopic theories of nuclei, such as the Strutinsky method, as well as in theories of nuclear matter in the bulk, relevant in astrophysical applications.

In nuclear physics, as well as in atomic and molecular problems, the following question often has to be answered: you are given a potential well, say a deformed Woods-Saxon potential, into which you put N quantized fermions into the lowest N eigenstates, up to a "Fermi energy" T_0. You square the wave functions of the particles and add them up to get the total density ρ:

$$\rho(\bar{r}) = \sum_{i}^{N} |\psi_i|^2 \quad .$$

Schematically the result looks something like Fig. 1.

<u>QUESTION</u>: Is there some simple way of estimating $\rho(\bar{r})$ without going through the misery of numerically solving N partial differential Schrödinger equations for the N particles?

2. THE STANDARD THOMAS-FERMI METHOD

The standard Thomas-Fermi method (e.g., Ref. 2) developed in the twenties for atomic problems and used extensively also in nuclear physics, gives an astonishingly simple answer:

$$\rho_{TF}(\bar{r}) \propto \begin{pmatrix} \textit{depth} \text{ of potential with} \\ \text{respect to Fermi energy} \end{pmatrix}^{3/2} ,$$

i.e.,

$$\frac{\rho}{\rho_0} \approx \left(\frac{T_0 - U}{T_0} \right)^{3/2} = (1-u)^{3/2} ,$$

where $u = U/T_0$, and ρ_0 is the central density. The quality of this approximation is illustrated in Fig. 2, which compares the exact (circles) and Thomas-Fermi (solid curve) densities in the surface region of a very large (semi-infinite) Woods-Saxon potential of depth 56 MeV filled with nucleons up to $T_0 = 37.76$ MeV (Ref. 3).

NOTE:

a) The Thomas-Fermi density has no wiggles (no Friedel oscillations).

More important:

b) The Thomas-Fermi surface profile is not very good, in particular ρ_{TF} cuts off to zero at the classical turning point of the top particle, where $T_0 - U$ turns negative and $(T_0 - U)^{3/2}$ becomes imaginary.

Thus: NO QUANTAL HALO in standard Thomas-Fermi. This is a fairly serious shortcoming since, in typical nuclei, of the order of 10% of the nuclear matter sits in the classically forbidden region. So: Thomas-Fermi is a fair approximation but needs improvement.

The topic of my talk is an improved Thomas-Fermi method which *does* give a quantal halo and a pretty accurate account of the surface profile (but still no wiggles).

3. THE MODIFIED THOMAS-FERMI METHOD

I give you at once the modified Thomas-Fermi equation for the density, and in the remainder of the time will describe as much of the physics and derivation as I can.

$$\text{Modified T.F.}\ \frac{\rho}{\rho_o} = \begin{cases} (1-u)^{3/2} & \text{for } \dfrac{\rho}{\rho_0} \geq 0.87 \\ C_1 e^{-u/c} - C_2 & \text{for } \dfrac{\rho}{\rho_0} \leq 0.87 \end{cases} \quad .$$

Here the constants C_1, C_2, c depend on the value of the separation energy S. (More precisely, on the dimensionless parameter of the problem, $\sigma \equiv S/T_0$.) This dependence is given by simple algebraic equations and is presented in Table I. The other curve in Fig. 2 shows how good the improved surface profile is.

4. THE PHYSICS OF THE MODIFIED METHOD

To explain the physics of the new scheme I have to remind you first of the physics of the standard Thomas-Fermi method. The key assumption of this method is that the kinetic energy of the quantized particles in the potential well can be written as an integral over all space of a *kinetic energy density* t, and that this t is proportional to the *five-thirds power of the density* ρ:

$$t \propto \rho^{5/3} \quad .$$

As is readily verified, this is the relation between t and ρ for a very large, *constant* potential well, i.e., for a very large box with a *flat* bottom filled with particles up to a Fermi momentum P_0, say.

PROOF: In momentum space the occupied quantum states fill a Fermi sphere of radius P_0. For a box of given size the density ρ is proportional to the total number of particles, which is proportional to the volume of the Fermi sphere:

$$\rho \propto P_0^3 \quad .$$

The energy per particles is proportional to P_o^2 (in fact equal to $(3/5)(P_o^2/2m)$ where m is the nucleon mass). Hence

t = energy density = (energy per particle $\propto P_o^2$)(density $\propto P_o^3$) $\propto P_o^5$.

$$\therefore \quad t \propto \rho^{5/3} , \quad QED \quad .$$

Let me write this as $t = (3/5)\ C\rho^{5/3}$, where C is a known constant, equal to $(3h^3/16\pi)^{2/3}/2m$ for standard nuclear matter.

In order to predict the T.F. density in a given potential $V(\vec{r})$, one now makes the total energy E stationary with respect to particle-preserving density variations $\delta\rho$:

$$\delta E = \underbrace{\int d^3x \left(V \right.}_{\substack{\text{change in} \\ \text{potential energy}}} + \underbrace{\left. \frac{dt}{d\rho} \right) \delta\rho}_{\substack{\text{change in} \\ \text{kinetic energy}}} = 0 \quad .$$

This leads to the Euler-Lagrange equation

$$\begin{aligned} V + C\rho^{2/3} &= \text{ constant Lagrange multiplier} \\ &= -\text{ separation energy } S \quad . \end{aligned}$$

Referring to Fig. 1 we find

$$\frac{\rho}{\rho_o} = \left(\frac{-V - S}{-V_o - S} \right)^{3/2} = \left(\frac{T_o - U}{T_o} \right)^{3/2} = (1-u)^{3/2}, \quad QED \quad .$$

So, the Thomas Fermi method is based on pretending that at each point the potential (and $\therefore$ density) are *flat*, which leads to

$$t \propto \rho^{5/3} \quad .$$

In the past 60 years countless papers have appeared on how to improve T.F. by going away from the flatness assumption, e.g., adding corrections to t, considered as an expansion in the *derivatives* of ρ:

$$t = \frac{3}{5} C\rho^{5/3} + \underbrace{k \frac{(\text{grad}\ \rho)^2}{\rho}}_{\text{"Weizsäcker correction"}} + \dots \quad .$$

This leads to so-called "Extended Thomas-Fermi Methods." These types of theories have been extremely successful, giving excellent systematic approximations to shell-averaged nuclear properties. Nevertheless, they have one practical drawback: one still needs to solve a (partial) differential equation to find $\rho(\bar{r})$ (because of the grad ρ in $t(\rho)$).

The modification I will describe takes a different tack: without introducing any gradients, it changes the function $t \propto \rho^{5/3}$ to something else, on physical grounds. The motivation is very simple: the function $\rho^{5/3}$ is always positive, and that is obvious nonsense in the low-density tail of a nuclear surface, where one is in the classically forbidden region. A particle in the classically forbidden region has a *negative* kinetic energy, so if one wants to capture the physics of that region one should make $t(\rho)$ negative for small ρ. Moreover, for very low ρ it is a trivial matter to write down the correct expression for $t(\rho)$. This is because the extreme density tail is dominated by the particles with the longest quantal tails, i.e., the particles at the top of the Fermi distribution, whose kinetic energy in the forbidden region is $-S$. It follows that the kinetic energy density there is $-S\rho$. Elementary! Thus

$$\boxed{t \rightarrow -S\rho} \quad \text{for} \quad \rho \rightarrow 0 \ ,$$

just by common sense. So we have this qualitative picture of $t(\rho)$: $\rho = (3/5)C\rho^{5/3}$ for $\rho \rightarrow \rho_o$, and $t(\rho) \rightarrow -S\rho$ for $\rho \rightarrow 0$. The question is then how to interpolate?

5. HOW TO INTERPOLATE?

I asked myself the following question: what function $t(\rho)$ would I need to insert in

$$\delta E = \int d^3x \left(V + \frac{dt(\rho)}{d\rho} \right) \delta\rho = 0$$

if I wanted to reproduce the *exact* (Durand et al.) density profile in Fig. 2? The function $\rho^{5/3}$ gives the poor T.F. profile, but if I change $\rho^{5/3}$ to something else, can I get the exact profile? The answer is yes, and it turns out that there is an elegant graphical construction which directly generates this $t(\rho)$ from the given $\rho_{\text{exact}}(x)$, at least apart from the Friedel wiggles, say for $\rho / \rho_o \leq 0.87$ (Ref. 1). The result is shown in Fig. 3. The upper curve is the T.F. kinetic energy density, the lower is the modified one that reproduces ρ_{exact} for $\rho / \rho_o \leq 0.87$ and joins on smoothly to t_{TF} at $\rho / \rho_o = 0.87$. There is a cute log-type parameterization of this curve:

$$\frac{t}{\rho_o T_o} \equiv \tau = \chi + c\left[(C_2 + \chi) \ln \frac{\chi + C_2}{C_1} - \chi - C_2 \ln \frac{C_2}{C1}\right]$$

designed so that when $t(\rho)$ is inserted in the variational equation $\delta E = 0$, it leads to the following simple equation for the density

$$\frac{\rho}{\rho_o} = C_1 e^{-u/c} - C_2 \ .$$

The three parameters C_1, C_2, c are determined uniquely by the three requirements that $t(\rho)$ should be equal to $t_{TF}(\rho)$ in value and slope at $\rho/\rho_o = \chi_1 = 0.87$, and that $t(\rho)$ should approach zero with slope $-S$ (i.e., $t \rightarrow -S\rho$ for $\rho \rightarrow 0$).

These three requirements can be shown to lead to the following algorithm relating C_1, C_2 and c to σ (= S/T_o): pick a value of C_2 and define B as χ_1/C_2, where $\chi_1 = 0.87$. Then c is given by $c = (2/5)\chi_1^{2/3} \Big/ \left[1 - \frac{\ln(1+B)}{B}\right]$, σ follows as $c\ln(1+B) - \chi_1^{2/3}$ and C_1 follows as $C_2 e^{(1+\sigma)/c}$. These equations have been used to generate Table I for C_1, C_2, and c in their dependence on σ.

Since the kinetic energy density is also given by a simple function of ρ, the energy of the system is also readily calculable.

This is only a little more laborious than the primitive T.F. scheme (no differential equations!), but gives a much better description of the surface profile, in particular it takes account of the classically forbidden region, the quantal halo.

6. AN APPLICATION

By glancing at Fig. 2 you will see that the principal effect of the modified method is to shift matter from the middle part of the surface profile, where the kinetic energy is positive, to the tail, where it is negative. This has a considerable effect on the kinetic energy contribution to the calculated surface energy, and even more on the kinetic energy part of the *curvature correction* to the surface energy. Thus if we were to write the total energy as

$$E = a_1 A + a_2 A^{2/3} + a_3 A^{1/3} + \cdots$$
$$= \left(a_1^{PE} + a_1^{KE}\right) A + \left(a_2^{PE} + a_2^{KE}\right) A^{2/3} + \left(a_3^{PE} + a_3^{KE}\right) A^{1/3} + \cdots \quad ,$$

with each coefficient split into contributions from the potential and kinetic energies, then from the example of Fig. 2 one can deduce (Ref. 1) that

$$a_1^{KE} = \frac{3}{5}(37.76) = 22.66 \text{ MeV}$$
$$a_2^{KE} = -18.15 \text{ MeV (OLD)} \rightarrow -26.89 \text{ MeV (NEW), i.e., } \Delta a_2 = -8.74 \text{ MeV}$$
$$a_3^{KE} = +5.9 \text{ MeV (OLD)} \rightarrow -11.0 \text{ MeV (NEW), i.e., } \Delta a_3 = -16.9 \text{ MeV} \quad .$$

This tendency of the quantal halo to lower a_3 drastically is a candidate for solving the so-called "curvature energy puzzle," i.e., the puzzle that many theoretical estimates (including standard T.F.) tend to predict $a_3 \approx 10$ MeV, whereas empirical evidence suggests $a_3 \approx 0$ MeV (Ref. 4).

To see whether this is indeed the answer we need to calculate a_3^{PE} in the old and new versions. Bill Myers and I are currently working on this problem.

ACKNOWLEDGMENTS

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Table I. The constants C_1, C_2 and c in the equation for the relative density, $\rho/\rho_0 = C_1 e^{-u/c} - C_2$, as functions of the relative separation energy $\sigma = S/T_0$.

σ	C_1	C_2	c	σ	C_1	C_2	c
0.00	1.38562	0.35936	0.74097	0.31	1.13464	0.06285	0.45276
0.01	1.36058	0.33218	0.71631	0.32	1.13289	0.06018	0.44970
0.02	1.33840	0.30791	0.69416	0.33	1.13126	0.05764	0.44678
0.03	1.31865	0.28615	0.67415	0.34	1.12974	0.05524	0.44398
0.04	1.30101	0.26653	0.65599	0.35	1.12832	0.05295	0.44131
0.05	1.28518	0.24879	0.63944	0.36	1.12699	0.05078	0.43874
0.06	1.27094	0.23267	0.62431	0.37	1.12574	0.04872	0.43629
0.07	1.25807	0.21799	0.61042	0.38	1.12458	0.04676	0.43394
0.08	1.24642	0.20457	0.59764	0.39	1.12349	0.04489	0.43168
0.09	1.23584	0.19227	0.58583	0.40	1.12246	0.04311	0.42952
0.10	1.22622	0.18097	0.57490	0.41	1.12151	0.04142	0.42744
0.11	1.21743	0.17056	0.56476	0.42	1.12061	0.03980	0.42544
0.12	1.20941	0.16094	0.55532	0.43	1.11977	0.03826	0.42353
0.13	1.20206	0.15205	0.54652	0.44	1.11898	0.03679	0.42168
0.14	1.19531	0.14380	0.53831	0.45	1.11824	0.03539	0.41991
0.15	1.18912	0.13614	0.53061	0.46	1.11754	0.03405	0.41820
0.16	1.18342	0.12901	0.52340	0.47	1.11689	0.03277	0.41656
0.17	1.17816	0.12237	0.51663	0.48	1.11628	0.03154	0.41498
0.18	1.17331	0.11616	0.51025	0.49	1.11571	0.03037	0.41345
0.19	1.16883	0.11037	0.50425	0.50	1.11518	0.02925	0.41198
0.20	1.16468	0.10494	0.49859	0.51	1.11467	0.02818	0.41057
0.21	1.16084	0.09986	0.49324	0.52	1.11420	0.02715	0.40920
0.22	1.15729	0.09508	0.48818	0.53	1.11376	0.02616	0.40788
0.23	1.15398	0.09060	0.48339	0.54	1.11334	0.02522	0.40661
0.24	1.15092	0.08638	0.47885	0.55	1.11295	0.02432	0.40538
0.25	1.14807	0.08241	0.47454	0.56	1.11259	0.02345	0.40420
0.26	1.14541	0.07867	0.47045	0.57	1.11225	0.02262	0.40305
0.27	1.14294	0.07514	0.46656	0.58	1.11193	0.02182	0.40194
0.28	1.14064	0.07180	0.46286	0.59	1.11163	0.02106	0.40087
0.29	1.13850	0.06865	0.45933	0.60	1.11135	0.02032	0.39984
0.30	1.13650	0.06567	0.45597				

FIGURE CAPTIONS

Fig. 1. A schematic illustration of wave functions in a potential well given by $U(\vec{r})$ or $V(\vec{r})$, and of the resulting total density $\rho(\vec{r})$.

Fig. 2. The relative density ρ/ρ_0 in a semi-infinite Woods-Saxon potential $u \equiv U/T_0$, where $U(x) = 56\ \mathrm{MeV}(1 + e^{-x/0.6\mathrm{fm}})^{-1}$.

Fig. 3. The relative kinetic energy density $\tau\,(\equiv t/\rho_0 T_0)$ is shown as a function of the relative density $\chi(\equiv \rho/\rho_0)$. The Thomas-Fermi curve is given by $(3/5)\chi^{5/3}$. The slightly modified energy density given by the lower curve (tending to $-\sigma\chi$ near the origin), when inserted in the Euler-Lagrange equation, leads to a close representation of the exact density profile in a typical surface potential.

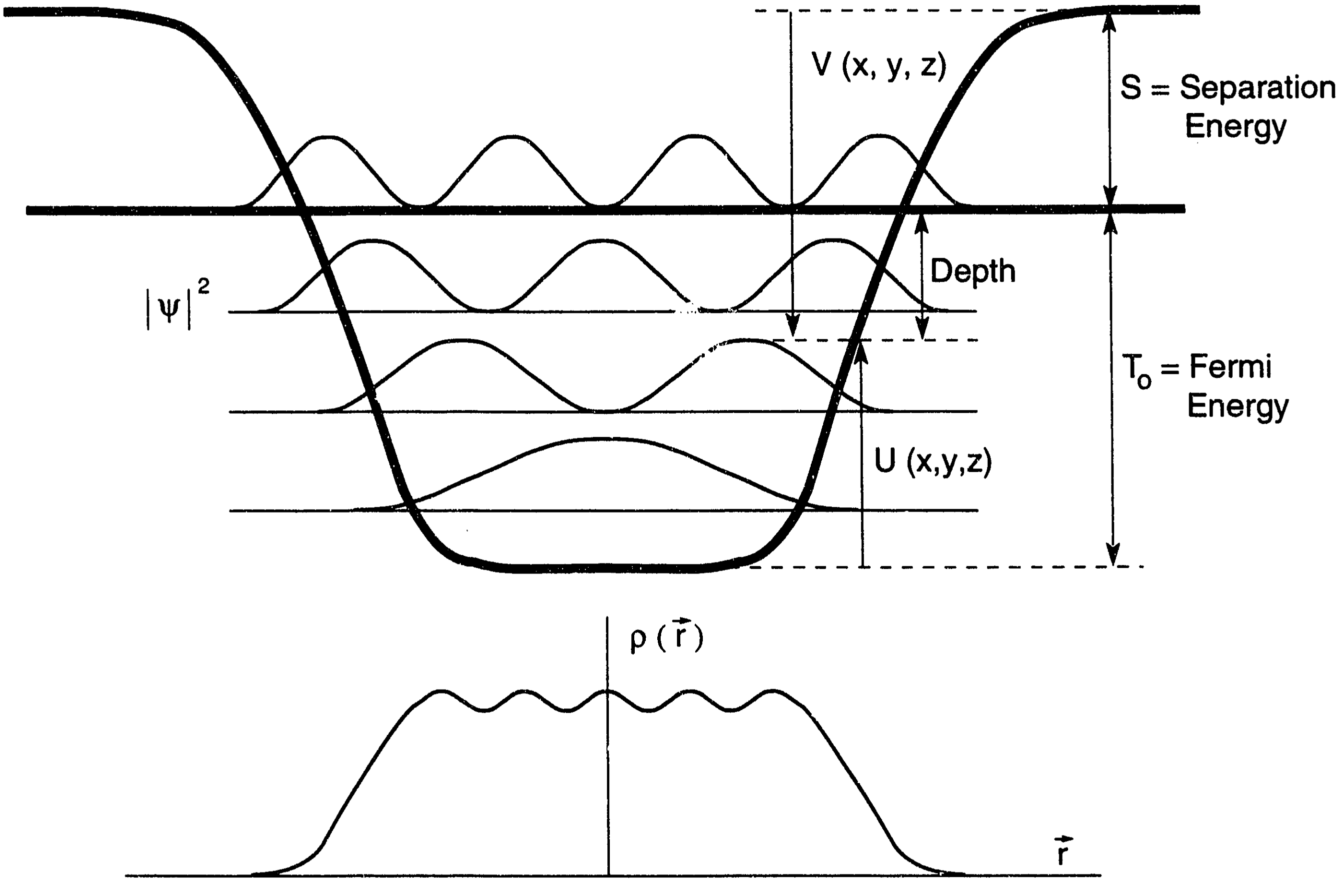

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Figure 1

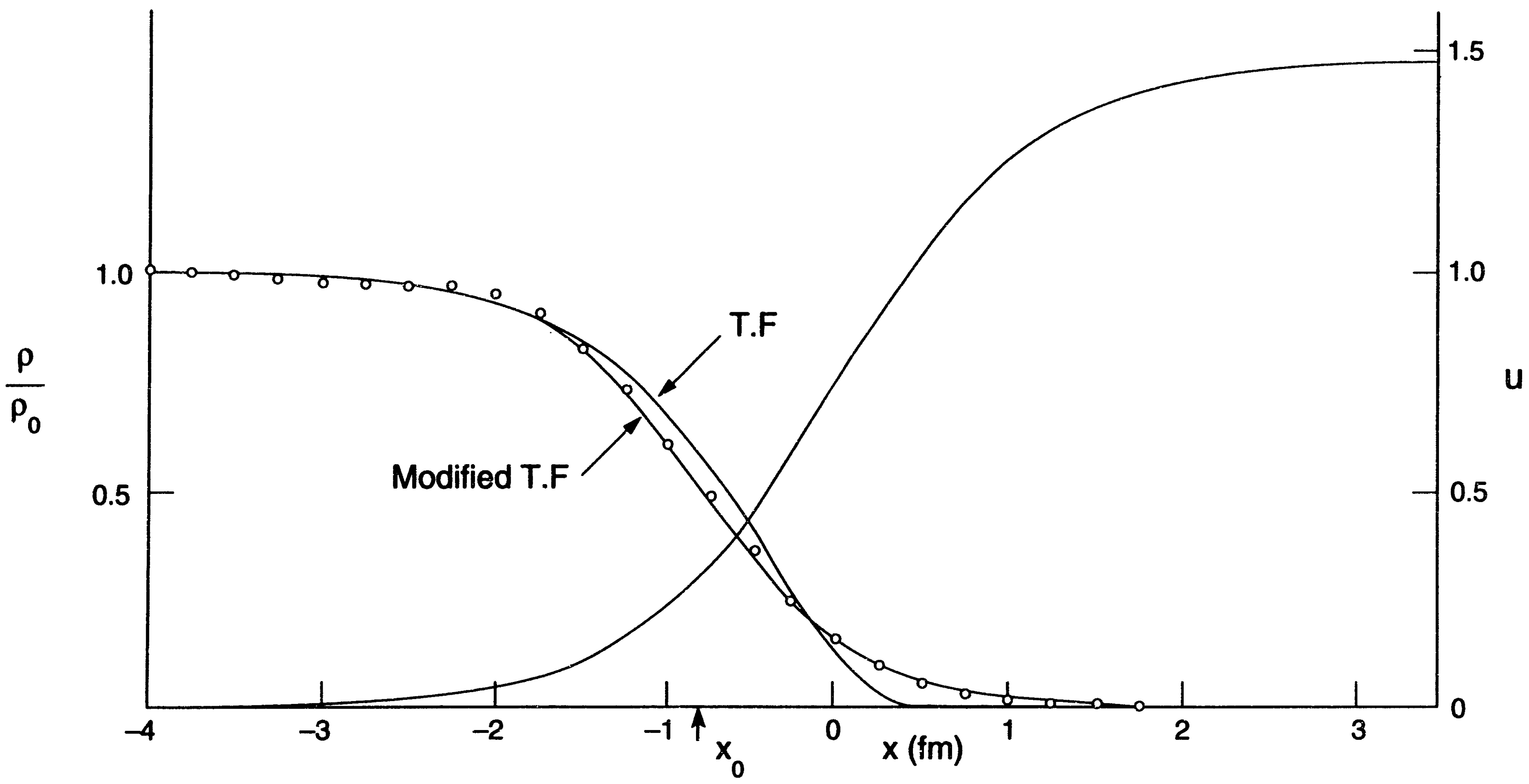

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Figure 2

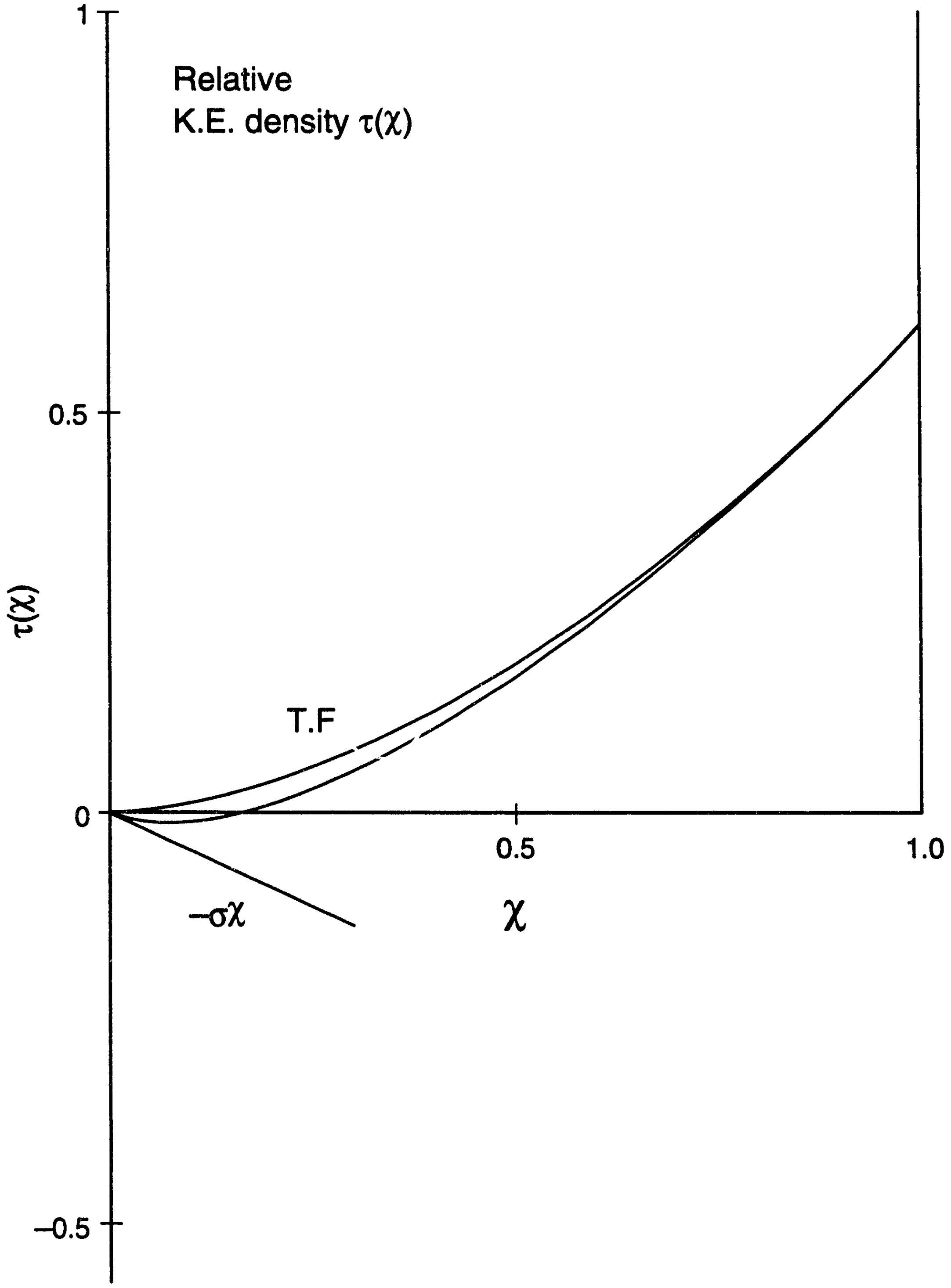

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Figure 3

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