TWO APPLICATIONS OF THE NUCLEAR THOMAS–FERMI MODEL* **

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We use the Thomas–Fermi model of macroscopic nuclear properties described in W.D. Myers and W.J. Swiatecki, *Nucl. Phys.* **A601**, 141 (1996), to discuss two applications: a) the response of the nuclear energy to changes of the neutron and proton diffusenesses, and b) the equation of state of cold nuclear matter. Under a) formulae are provided which will make it possible to improve existing Microscopic–Macroscopic calculations of nuclear properties by the inclusion of the two degrees of freedom associated with the neutron and proton diffusenesses. The algebraic formulae presented under b) may serve as a reliable baseline estimate of the equation of state. It is argued that the value of the nuclear compressibility coefficient K as well as its dependence on the relative neutron excess are now fairly well determined.

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1. Introduction

Since the discovery of the nuclear independent-particle model in 1949 the starting point of most nuclear theories involves the solution of the wave equation of non-interacting particles in a common potential. The potential may be taken to have some reasonable-looking Woods–Saxon-like shape, but today's computers are sufficiently powerful so that the potential can be generated self-consistently by the nucleons themselves, assumed to be interacting by some effective force. Thus one achieves the solution, in the

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mean-field approximation, of an idealized many-body problem of interacting nucleons. These are the Hartree–Fock theories, recently generalized into the form of relativistic mean-field treatments.

If, following Thomas and Fermi, one makes the additional, standard statistical approximation of averaging over shell effects ("two fermions per h^3 of phase space") one arrives at the Thomas–Fermi self-consistent mean-field solution of the nuclear many-body problem, Ref. [1].

In both the Hartree–Fock and Thomas–Fermi approximations a central problem is to invent an appropriate effective interaction that will mock up adequately the physics of the true, unapproximated many-body situation. A more technical difficulty is to achieve a sufficiently precise adjustment of the effective interaction's half dozen parameters to the couple of thousand measured binding energies and other relevant nuclear properties.

Table I, based on Ref. [2], compares the quality of the fits to nuclear masses for 17 current models: ten Hartree–Fock calculations with various Skyrme or Gogny forces, three relativistic models and four hybrid "Macroscopic-Microscopic" approaches. What is shown is the RMS deviation, in MeV, between theory and measurement for a sample of 116 spherical even-even nuclei from ^{16}O to ^{220}Th. The Thomas–Fermi model, which is the subject of this talk, is labeled MM(TF) in Table I. Its macroscopic part is the shell-averaged, self-consistent mean-field solution of A nucleons interacting by an effective velocity- and density-dependent Yukawa potential. The interaction has 6 adjustable parameters, which were fitted to 1654 measured masses of nuclei with $N, Z > 8$, as well as to the diffuseness of the nuclear surface. The adjustment to masses was made after these were smoothed by subtracting Strutinsky shell effects, an empirical even-odd correction and a semi-empirical Congruence (Wigner) term. These corrections are beyond a statistical treatment, and have to be addressed separately (hence the appellation "Macro-Micro"). The RMS deviation for this hybrid Thomas–Fermi model is 0.57 MeV for the 116 masses on which Table I is based, and 0.655 MeV for the full set of 1654 masses. Most of this 0.655 MeV is readily recognized as to due imperfections in the microscopic shell corrections. Thus, recalling that for a medium mass nucleus the binding energy is some 1000 MeV, one is talking about a precision in the fit to the macroscopic part of the energy of the order of 1 in 10^4.

A feature that sets the Thomas–Fermi model apart from most of the models in Table I is that, without any readjustment of the parameters, it gave a good account (apart from indications of slight overestimates in the mass range $A = 75$ to 98) of the 40 measured fission barriers of nuclei throughout the periodic table. This is a severe test of a model's deformability properties, since saddle-point shapes defining the fission barriers are very strongly deformed configurations.

TABLE I

Mass rms deviations in MeV

SIII:	4.74	SkP:	2.37	SkM*:	6.32	
SIII^{δ}:	3.07	SkP^{δ}:	2.53	$\mathrm{SkM}^{*\delta}$:	5.36	HARTREE–FOCK
$\mathrm{SIII}^{\delta\rho}$:	2.26	$\mathrm{SkP}^{\delta\rho}$:	2.32	$\mathrm{SkM}^{*\delta\rho}$:	4.74	
Gogny:	2.07					
RMF(NL1):	3.94	RMF(NL2):	11.24	RMF(NL3):	2.48	RELATIVISTIC
ETFSI:	0.80					
MM(FRDM):	0.65	MM(FRLDM):	0.76	MM(TF):	0.57	MACRO–MICRO

The model passed three additional tests, again without the readjustment of parameters: the masses of light nuclei with $N, Z < 8$, not included in the fit, came out reasonably close to measurements, nuclear sizes were predicted correctly, and the density dependence of the energy of neutron matter came out close to the theoretical estimates of Ref. [3].

The good agreement with shell-corrected nuclear masses and the satisfactory outcome of the above four tests makes us feel that the Thomas–Fermi model provides not only an accurate representation of the macroscopic properties of known nuclei, but can also serve as the basis for extrapolating these properties to unknown regions of the chart of nuclei, as well as to nuclear matter.

We have already used our model in a number of applications (Refs. [1,4,5]), and in what follows I will describe two recent examples.

2. The nuclear surface diffuseness as a degree of freedom

Estimating the dependence of the nuclear surface energy on surface diffuseness may turn out to be important for locating more reliably the magic numbers in the region of superheavy nuclei. Thus in macroscopic-microscopic approaches to extrapolations into the superheavy regime, the nuclear mean field is parameterized as a shape-dependent Woods–Saxon or similar potential, in which the Strutinsky shell corrections are then evaluated. In order to find the ground-state energy and shape of the nucleus, in particular a super-heavy nucleus, the sum of the microscopic shell correction and a macroscopic energy is varied as a function of the shape degrees of freedom. In such variations the surface diffuseness is usually kept constant, but one may well ask how the results would change if, when locating the energy minimum, the diffuseness were to be treated as an additional degree of freedom, to be varied simultaneously with the shape degrees of freedom. This question has, in fact, a long history going back at least to Refs. [6,7,8]. There have also been indications as long ago as 1966 (see Fig. 4 in [9]), that an increased surface diffuseness would begin to favour the magic proton number $Z = 126$ over 114. This possibility has been examined in the recent comprehensive study in [10], where macroscopic-microscopic extrapolations were confronted with self-consistent Hartree–Fock calculations, in which the mean field is not parameterized, but is allowed to seek out its optimum form, including whatever changes in the surface diffuseness are called for.

The resulting possibility of a reappearance of the magic number $Z = 126$ would affect profoundly forthcoming searches for superheavy nuclei, and it is important to throw further light on this question by performing up-to-date macroscopic-microscopic calculations generalized to include the surface degrees of freedom. In order to carry out such a calculation it is necessary to investigate the response to diffuseness of both the macroscopic and microscopic parts of the energy. The machinery for calculating the latter is already in place: simply recalculate the Strutinsky shell correction for a series of diffusenesses. As regards the former a new question arises: besides the known response of the Coulomb energy to diffuseness, one needs the response of the macroscopic surface-layer energy. Here is what the Thomas–Fermi model has to say about this [11].

Consider a finite nucleus with mass number A (and $N = Z$), for which the surface diffuseness for neutrons is λ_n times (and for protons λ_p times) what it would be for standard, semi-infinite nuclear matter. A series of numerical solutions of the Thomas–Fermi equations shows that the sum of surface and curvature energies in their dependence on λ_n and λ_p can be approximated by

$$\begin{aligned} E \;=\; & S\left[1 + \tfrac{1}{2}\phi_1(\lambda_n - 1)^2 - \phi_2(\lambda_n - 1)(\lambda_p - 1) + \tfrac{1}{2}\phi_1(\lambda_p - 1)^2\right] \\ & + K\frac{\lambda_n + \lambda_p}{2} \\ & + \text{cubic terms in } (\lambda_n - 1), (\lambda_p - 1)\,, \end{aligned} \tag{1}$$

where

$$S = 18.63 A^{2/3}\,\text{MeV}, \quad K = 12.11 A^{1/3}\,\text{MeV} \tag{2}$$

are the Thomas–Fermi model's standard surface and Coulomb energies for $\lambda_n = \lambda_p = 1$. For $A > 40$ the coefficients ϕ_1 and ϕ_2 are given approximately by the following functions of A:

$$\phi_1 = 0.7388 + 1.1787\alpha + 12.5929\alpha^2\,, \tag{3}$$

$$\phi_2 = 0.4836 + 0.4178\alpha + 5.2180\alpha^2\,, \tag{4}$$

with $\alpha = A^{-1/3}$.

For a spherical nucleus with atomic number Z the Coulomb energy may be written as an expansion in the ratio of the diffuseness to the effective sharp radius R and, using standard formulae [12], one finds

$$E_C = C - C_2\lambda_p^2 + C_3\lambda_p^3\,, \tag{5}$$

where

$$C = \frac{3e^2Z^2}{5R} = \frac{0.7579Z^2}{A^{1/3}} \quad \mathrm{MeV}\,, \tag{6}$$

$$C_2 = \frac{3e^2Z^2w_0^2}{2R^3} = \frac{1.4579Z^2}{A} \quad \mathrm{MeV}\,, \tag{7}$$

$$C_3 = \frac{3e^2Z^2w_0^3k_3}{5R^4} = \frac{1.5457Z^2}{A^{4/3}} \quad \mathrm{MeV}\,. \tag{8}$$

Here e is the charge unit and k_3 is a numerical coefficient which, for a Fermi function charge distribution, has the value 3.0216. The quantity w_0 is a measure of the diffuseness for standard semi-infinite nuclear matter and has the approximate value $w_0 = 1$ fm. We also took $R = 1.14A^{1/3}$ fm.

Adding Eq. (5) to Eq. (1) and minimizing with respect to λ_n and λ_p one finds for the optimum value of λ_p the relation

$$\lambda_p = \frac{\sqrt{c_1^2 + 4c_0c_2} - c_1}{2c_2}\,, \tag{9}$$

where

$$c_0 = 1 - \frac{K}{2S\chi} = 1 - \frac{0.3250}{A^{1/3}\chi}\,, \tag{10}$$

$$c_1 = 1 - \frac{2C_2}{S\psi} = 1 - \frac{0.1565Z^2}{A^{5/3}\psi}\,, \tag{11}$$

$$c_2 = \frac{3C_3}{S\psi} = \frac{0.2489Z^2}{A^2\psi}\,, \tag{12}$$

where ψ stands for$(\phi_1^2 - \phi_2^2)/\phi_1$ and χ stands for $(\phi_1 - \phi_2)$.

The optimum value of λ_n is related to λ_p by

$$\lambda_n - 1 = \frac{\frac{-K}{2S} + (\lambda_p - 1)\phi_1}{\phi_2} = \frac{-0.3250A^{-1/3} + (\lambda_p - 1)\phi_1}{\phi_2}\,. \tag{13}$$

Figure 1 compares the predicted values of the relative diffuseness λ_p with measured relative diffusenesses, obtained by taking the values of the diffuseness parameter "z" for $A \geq 40$, listed in Ref [13] for "two-parameter

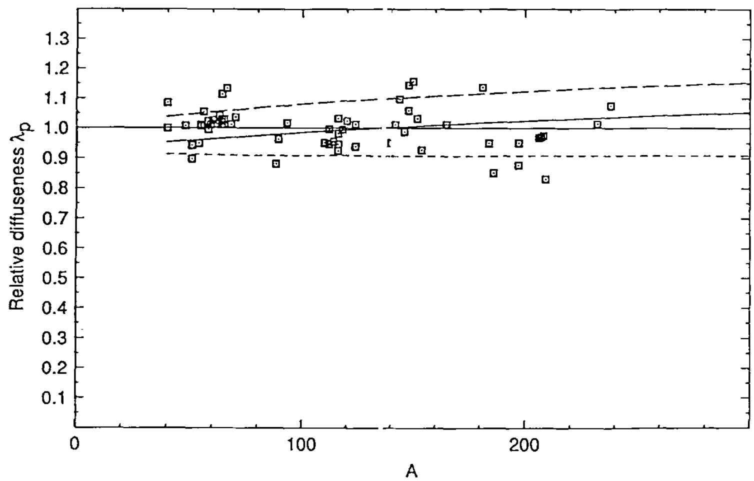

Fig. 1. The solid curve is the relative proton diffuseness λ_p as predicted by Eq. (9) along the valley of stability. The long-dashed curve shows the result of disregarding the curvature energy, the short-dashed curve the result of disregarding the Coulomb energy. The squares refer to the relative proton diffuseness deduced from measurements of charge distributions according to [13].

Fermi fits," and dividing them by their average (equal to about 1.022 fm). It will be seen that, along the valley of stability, theory predicts a slight gradual increase of the diffuseness, the result of the competition of Coulomb and curvature driving forces pushing against the surface-energy restoring potential. For the super-heavy nucleus $Z = 126$, $N = 184$ (which is off the valley of stability) Eq. (9) gives $\lambda_p = 1.081$ as the optimum diffuseness. The cost of a further increase of λ_p from the optimum (assuming, for purposes of illustration, that the changes in neutron and proton diffusenesses are locked in step) is found by taking the second derivative of Eq. (1) with $\lambda_n = \lambda_p = \lambda$:

$$\Delta E = \frac{1}{2}\frac{d^2E}{d\lambda^2}(\lambda - 1)^2 = 411.5(\lambda - 1)^2\,\mathrm{MeV}\,. \tag{14}$$

For example, an additional 10% increase of diffuseness would cost about 4 MeV. It remains to be seen whether the possible gain in shell-effect energy associated with making the nuclear potential more oscillator-like (which is estimated both in Ref. [8] and [10] as up to a dozen MeV) would be able to stabilize the above super-heavy nucleus sufficiently to make it detectable. The problem is under study, Ref. [14]. However this will turn out, it is now possible to improve the conventional macroscopic-microscopic method by including the degrees of freedom associated with the neutron and proton diffusenesses. This may lead to a better description of nuclear masses and deformation energies throughout the periodic table, especially near the drip lines. It may also be useful in macroscopic descriptions of the giant monopole resonance.

3. The nuclear equation of state

There is currently considerable interest in the energy per particle of nuclear matter, $e(\rho, \delta)$ considered as a function of the nuclear density ρ and the relative neutron excess δ, where $\rho = \rho_{\text{neutrons}} + \rho_{\text{protons}}$ and $\delta = (\rho_n - \rho_p)/\rho$. This fundamental quantity, the equation of state of cold nuclear matter, plays a key role in theories of neutron stars and supernova explosions, as well as in the interpretation of nucleus-nucleus collisions at energies where nuclear compressibility comes into play. (For a review and references see, for example, Ref. [15].)

Direct information on $e(\rho, \delta)$ is difficult to come by for values of ρ away from those characterizing normal nuclei and for δ beyond the relatively small values characteristic of the most neutron-rich nuclei. One way to extrapolate beyond this limited regime is by using a nuclear model fitted to binding energies of finite nuclei and extrapolating to nuclear matter. Having developed a reliable Thomas–Fermi model of finite nuclei we can readily make this extrapolation, and this is what we find:

$$e(\rho, \delta) = T_0 \eta(\Omega, \delta)\,,$$

where

$$\eta(\Omega, \delta) = a\Omega^2 - b\Omega^3 + c\Omega^5\,. \tag{15}$$

Here $\Omega \equiv (\rho/\rho_0)^{1/3}$ and $\rho_0 = 0.16114\,\text{fm}^{-3}$ and $T_0 = 37.0206$ MeV are the saturation density and Fermi energy of standard nuclear matter as predicted by the model. The coefficients a, b, c are the following functions of δ:

$$a = \frac{3}{20}\left[2(1-\gamma_l)(p^5+q^5) - \gamma_u \begin{cases} (5p^2q^3 - q^5) & \text{for } \rho_n \geq \rho_p \\ (5p^3q^2 - p^5) & \text{for } \rho_n \leq \rho_p \end{cases}\right], \tag{16}$$

$$b = \frac{1}{4}\left[\alpha_l(p^6+q^6) + 2\alpha_u p^3 q^3\right] \tag{17}$$

$$c = \frac{3}{10}\left[B_l(p^8+q^8) + B_u p^3 q^3 (p^2+q^2)\right], \tag{18}$$

where $p = (1+\delta)^{1/3}, q = (1-\delta)^{1/3}$. The quantities $\gamma_l, \gamma_u, \alpha_l, \alpha_u, B_l, B_u$ are relative interaction strengths characterizing the effective nucleon–nucleon force in the Thomas–Fermi model. They have the following values

$$\begin{aligned} \gamma_l &= 0.25198\,, & \gamma_u &= 0.88474\,,\\ \alpha_l &= 0.70110\,, & \alpha_u &= 1.24574\,,\\ B_l &= 0.22791\,, & B_u &= 080020\,. \end{aligned} \tag{19}$$

Figure 2 displays the dimensionless energy per particle $\eta(\Omega, \delta)$ as a function of Ω for $\delta = 0, 0.2, 0.3, 0.4, \ldots 1.0$. It will be seen that neutron matter ($\delta = 1$) is unbound in our model. A minimum in η appears below the critical value $\delta_c = 0.8213$, where $\Omega = \Omega_c = 0.5735$ and $\eta_c = 0.02979$. The saturation energy per particle becomes negative for $\delta < 0.7783$ and attains the value $\eta = -0.43859$ (*i.e.*, $e = -16.24$ MeV) at $\delta = 0$. Figure 2 shows, as a function of δ, the density ρ, the energy per particle e, and the compressibility K_0 along the sequence of minima in Fig. 2.

The equilibrium value of Ω is obtained by solving the cubic resulting from equating to zero the derivative $\partial\eta/\partial\Omega$ which leads to $\Omega = 0$ or

$$2a - 3b\Omega + 5c\Omega^3 = 0\,. \tag{20}$$

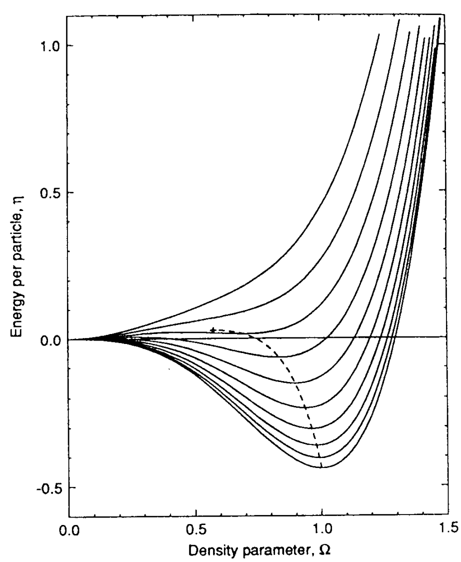

Fig. 2. The dimensionless energy per particle $\eta(\Omega, \delta)$ plotted as function of Ω, the cube root of the relative density ρ/ρ_0, for ten values of the relative neutron excess $\delta = 0, 0.2, 0.3, 0.4, \ldots, 1.0$. The dashed curve follows the loci of the energy minima up to the critical point marked by a cross.

The relevant solution is

$$\Omega = \sqrt{\frac{b}{5c}} \left[\cos\frac{\theta}{3} + \sqrt{3}\sin\frac{\theta}{3} \right] , \tag{21}$$

where

$$\theta = \cos^{-1}\left(ab\sqrt{\frac{5c}{b}} \right) . \tag{22}$$

The compressibility coefficient at the minimum, K_0, is given by

$$K_0(\delta) = 9\left[\rho^2 \frac{\partial^2 e}{\partial \rho^2} \right]_{\rho=\rho_{\min}} = T_0(2a\Omega^2 - 6b\Omega^3 + 20c\Omega^5) , \tag{23}$$

with Ω given by Eq. (21).

As can be seen from Fig. 3, K_0 starts at 234 MeV at $\delta = 0$ and decreases to zero at the critical point δ_c. Figure 3 shows also that the behaviour of $K_0(\delta)$ parallels the behaviour of the depth of the binding energy minimum taken with respect to the energy e_c at δ_c. This is an extension to large values of δ of the parallelism between $K(N, Z)$ and $e(N, Z)$ for finite nuclei, discovered in Refs. [16,17]. This near constancy of the ratio of compressibility to binding energy is illustrated by the fact that this ratio changed by only 7.5% between $\delta = 0$ and $\delta = 0.52$, where e was halved from -16.24 MeV to -8.12 MeV.

In some applications the compressibility of nonequilibrium nuclear matter is of interest. Defining $K(\rho, \delta)$ in the usual way as

$$K(\rho, \delta) = 9\frac{\partial P}{\partial \rho} , \tag{24}$$

where P is the pressure given by $P = \rho^2(\partial e/\partial \rho)$, we find

$$K(\rho, \delta) = T_0(10a\Omega^2 - 18b\Omega^3 + 40c\Omega^5) . \tag{25}$$

This is again readily evaluated for a given δ by calculating the coefficients a, b, c, using Eqs. (16)–(18).

Equation (15) represents the extrapolated equation of state as predicted by a model that gives the currently most accurate representation of measured binding energies and fission barriers [1,2,4]. For relatively modest deviations from standard density, the key quantity is the compressibility $K_0(\delta)$, whose value at $\delta = 0$ we estimate as about 234 MeV. Other recent estimates of this quantity [18,19], based on the interpretation of the giant monopole resonance, suggest values near 215 MeV. At the present time there is enough

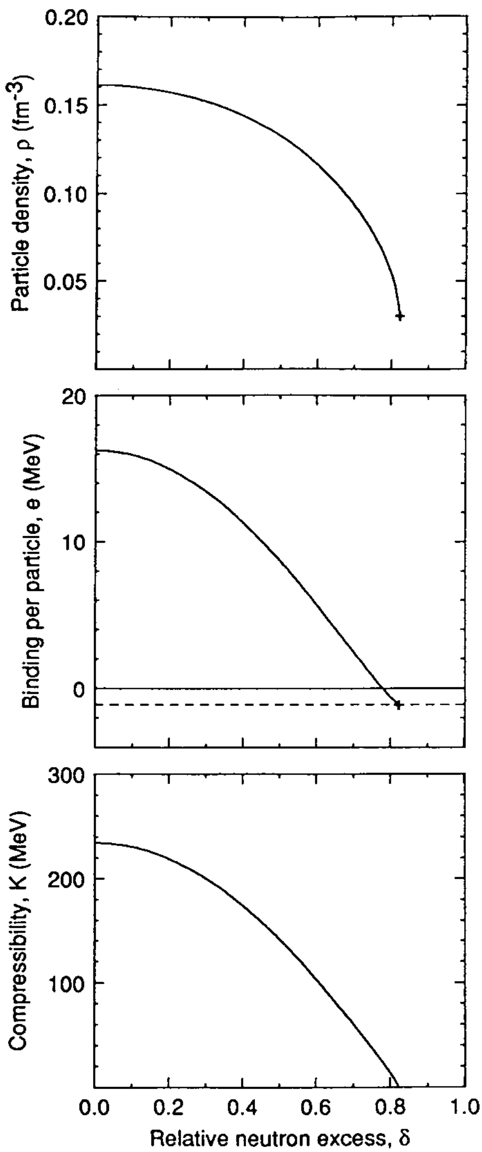

Fig. 3. The saturation density ρ, the energy per particle e and the compressibility $K_0(\delta)$ at saturation, plotted as function of the relative neutron excess δ. The compressibility vanishes at the critical point defined by $\delta_c = 0.8213$, where $\rho_c = 0.03039\ \mathrm{fm}^3$ and $e_c = 1.1029$ MeV. Note the similarity of the δ dependences of K_0 and $e_c - e$. (The dashed line corresponds to $e = e_c$.)

uncertainty all around so that we do not regard this 8% difference as necessarily significant. But the relative reliability of estimates of K_0 derived from a very precise fit of a nuclear model to binding energies and the surface diffuseness does not appear to be sufficiently appreciated. Thus one still finds statements to the effect that the saturation energy and density are the only well determined characteristics of the equation of state, and compressibility coefficients differing by a factor of two are quoted in the literature. We believe that the Thomas–Fermi model has reduced the uncertainty concerning the value of K being around 230 MeV, and that the value derived from giant monopole resonances is in substantial agreement with this conclusion. We also believe that the dependence of the compressibility on neutron excess predicted by Eq. (23) is fairly reliable.

For very large extrapolations (several times the standard density) our simple expression for $e(\rho,\delta)$ will have to be judged by whatever experimental information becomes available, and by comparisons with theories that are considered to be intrinsically more reliable. (In this connection see Ref. [20], where our $e(\rho,\delta)$ was incorporated in neutron star studies and the results compared with those based on other theoretical equations of state.) In the meantime, because of its simplicity and firm contact with measured properties of finite nuclei, our algebraic expression for $e(\rho,\delta)$ could be used as a convenient baseline formula for the equation of state of cold nuclear matter.

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