SEMICLASSICAL CALCULATIONS OF NUCLEAR GROSS PROPERTIES WITH SKYRME INTERACTIONS [+)]

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Abstract

We present the results of calculations of nuclear ground state properties and fission barriers using the semiclassical (ETF) energy density formalism. Realistic average barrier heights are obtained with the Skyrme force SkM. Relations to droplet model parameters are discussed and their systematic determination using the leptodermous approximation is explicitly demonstrated and justified also for deformed nuclei.

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I. Introduction

We have recently shown [1] that the energy density method using realistic Skyrme forces can successfully be used to calculate not only average nuclear ground state properties such as binding energies, densities and radii, but also fission barriers which are in close agreement with the averaged part of Hartree-Fock (HF) results. An important ingredient hereby are the ETF(Extended Thomas-Fermi) functionals for the kinetic energy and spin-orbit densities, in which contributions from orders up to $\hbar^4$ in the semiclassical expansion must be included in order to correctly describe deformation energies [2,3].

In section II we shall present the newest results of these calculations, emphasizing in particular the fission barriers obtained with different Skyrme forces for the standard test nucleus Pu^{240}. The deformation energies are analyzed in terms of surface, curvature and Coulomb energy contributions to make contact with liquid drop and droplet model parametrizations. We shall show that, in fact, the results of our variational calculations are compatible with the droplet model [4] relations if a non zero curvature energy coefficient is allowed for.

In section III we show explicitly how, using a suitable coordinate system adapted to the nuclear deformation, the symmetric liquid drop(let) parameters can easily be determined very accurately using the leptodermous expansion. The latter is demonstrated to work well even beyond actinide saddle point configurations. The dependence of the central nuclear density on incompressibility, surface and curvature energy coefficients is worked out and the A dependence of the incompressibility is discussed for a model Skyrme force (SVII).

II. Results for ground state properties and fission barriers

Our goal being: (i) To calculate the average part of the deformation energy along the fission path with an accuracy of the order of 1 MeV,

(ii) to compare it to the mean HF value obtained with the same force,

(iii) not to use other extra parameters than those of the force adjusted in a HF calculation,

we use the ETF approximation. In order to fulfill the above requirements, we showed in a previous paper [2] that it is necessary to consider the 4th order terms in the expansion of nucleon and kinetic energy densities in powers of $\hbar$. In fig. 1 we recall our results obtained with deformed harmonic oscillator densities. There the following routine was adopted:

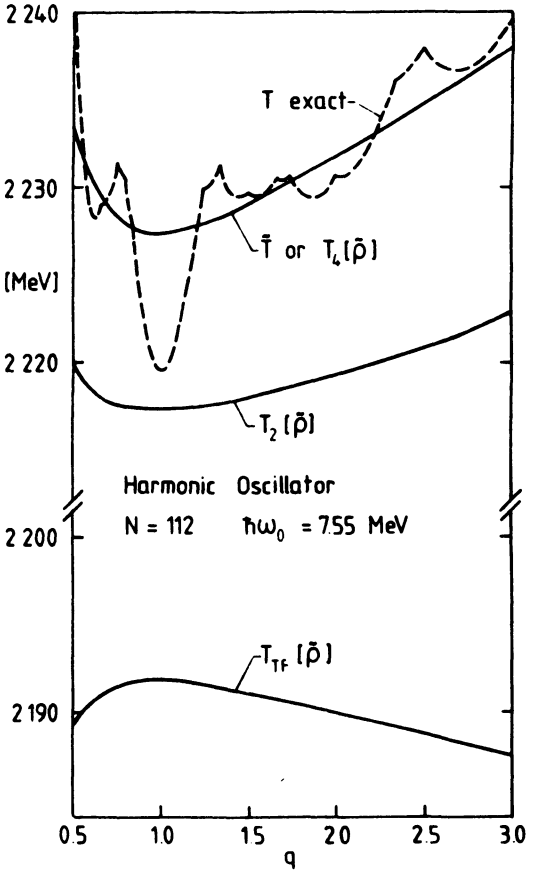

Fig. 1

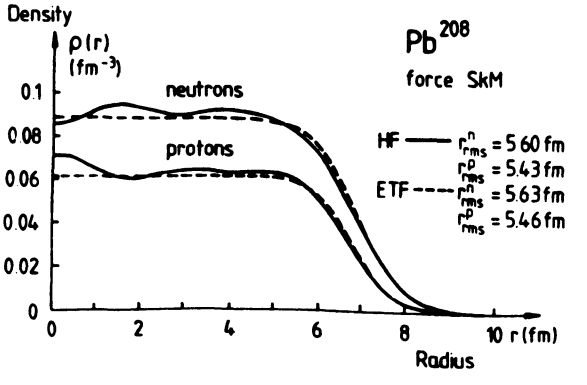

Fig. 2

Start from the Strutinsky averaged density

$$\tilde{\rho}(\vec{r}) = \sum_i |\varphi_i(\vec{r})|^2 \tilde{n}_i ,$$

compare the ETF kinetic energy (density)

$$T_{ETF} = \frac{\hbar^2}{2m} \int \tau_{ETF}[\rho] \, d^3r ,$$

(where $\tau_{ETF}[\rho]$ is the functional containing derivatives of ρ up to order 4) to the Strutinsky averaged kinetic energy (density):

$$\tilde{T} = \frac{\hbar^2}{2m} \int \tilde{\tau}(\vec{r}) d^3r = \frac{\hbar^2}{2m} \int \sum_i |\vec{\nabla}\varphi_i(\vec{r})|^2 \tilde{n}_i \, d^3r .$$

Even for large deformations (as encountered in fission) the agreement between these 2 quantities is within the Strutinsky plateau uncertainty ($\sim$1MeV). The local validity of the ETF functional was also investigated and its ability to describe the surface was found to be very good [2] . This aspect has then been extensively studied in realistic calculations; a typical example is shown in fig. 2. Here we compare the proton and neutron density profiles for ^{208}Pb as obtained with the functional, to the exact HF ones for the force SkM [5] . As in all calculations presented below, we use the full 4th order ETF functional as derived by Grammaticos and Voros [6] , i.e. for the general case including effective mass and spin orbit potentials. The semi-classical solution has been obtained by restricting the variational problem (Euler Lagrange equation) to a minimization of the total energy in a limited space spanned by Fermi-functions, which means a minimization with respect to two parameters (for protons and neutrons each), namely the central density and the surface diffuseness. This simple choice has been tested and justified by considering somewhat more complicated functions such as:

$$\rho(r) = \frac{\rho_0}{\left\{1 + \exp\left(\frac{r-R}{\alpha}\right)\right\}^\beta} \left[1 + w\left(\frac{r}{R}\right)^2\right] .$$

The gain in binding energy, for a heavy system, is then less than 3 MeV (to be compared to about 1500 - 2000 MeV). Other radial shapes were also tried and found to be worse than the Fermi-function.

The outer part of the HF surface tail is surprisingly well reproduced. This success could not be reached without the inclusion of the 4th order terms in the functional. Attempts had been made by other authors [5,7] to simulate these higher order effects by readjusting the Weizäcker coefficient, but this lead to a less nice reproduction of the outer tail and furthermore is not applicable for deformation energies. The somewhat less good agreement in the inner part of the surface is probably due to our restricted choice of a Fermi-function. That the surface region is well described, gives us confidence in this method for describing a process such as fission which is sensitive to the rearrangements in the surface.

Before proceeding to this subject, let us compare the binding energies and radii from HF and semi-classical calculations. Table 1 shows results obtained

Nucleus	B^{EXP}	B^{HF}	B^{ETF}	r_c^{EXP}	r_c^{HF}	r_c^{ETF}	$(r_n-r_p)^{HF}$	$(r_a-r_p)^{ETF}$	α_n	α_p
^{16}O	127.6	131.5	116.9	2.73	2.79	2.78	- 0.03	- 0.03	0.450	0.443
^{40}Ca	342.1	347.9	333.3	3.49	3.50	3.45	- 0.04	- 0.04	0.448	0.458
^{48}Ca	416	428.1	412.6	3.48	3.52	3.52	0.16	0.17	0.491	0.431
^{56}Ni	484.	495.5	477.8	3.75	3.75	3.79	- 0.05	- 0.05	0.451	0.462
^{90}Zr	783.9	794.8	782.9	4.27	4.28	4.27	0.07	0.08	0.478	0.442
^{114}Sn	971.6	975.2	971.7		4.60	4.59	0.08	0.08	0.482	0.440
^{132}Sn	1102.7	1123.7	1107.6		4.71	4.73	0.24	0.25	0.527	0.425
^{140}Ce	1172.7	1180.8	1174.8	4.88	4.89	4.87	0.14	0.14	0.499	0.433
^{280}Pb	1636.5	1652.7	1636.7	5.50	5.49	5.52	0.18	0.17	0.513	0.426

Table 1: The semiclassical binding energies, B^{ETF}, contain shell-effects.

for some spherical nuclei with the force SkM. Since the semi-classical binding energies do not contain shell fluctuations, a comparison with HF values cannot be straightforward. However, we picked up shell corrections from a table and added them to the semi-classical values. For the charge radii, we took into account the same Gaussian proton form factor as in the HF calculations. Both on radii and binding energies, the agreement is seen to be very good. It is worth noting that the semiclassical values are closer to the experimental ones than the HF values for the special case of the force SkM considered here. As a matter of fact, the mean deviation is about 3 MeV all over the range considered here. For a more comprehensive analysis of the properties of the SkM force see the contribution of P. Quentin in this meeting and a forthcoming paper [8]. In table 1 one also reads the diffuseness parameters of the best Fermi-function. Clear isospin effect is observed depending essentially on the compressibility of the force and is present for any Skyrme force (see ref. [17]). The neutrons experience a more diffuse surface, although the Coulomb force would tend to counteract this effect, as seen for the symmetric nuclei. Note also that the proton skin thickness stays almost constant in agreement with experimental observations.

In order to study deformed nuclear density distributions, we use an "intrinsic" coordinate system which will be described in the next section. The half density surface is parametrized according to the $\{c,h\}$ prescription of ref. [9] which is known to be adequate for typical saddle-point deformations of actinides. Using the SIII force we show in fig. 3 how the full inclusion of 4th order terms (curve SC4) provides a liquid drop fission barrier close to the average part of the HF curve, whereas a restriction to only 2nd order terms would have led to a large underestimation of the barrier height. Our results show in an independent way that the well-known defect of the HF-Skyrme calculation of fission barriers [10] has to do with the force itself rather than with technical problems associated to the HF method such as basis

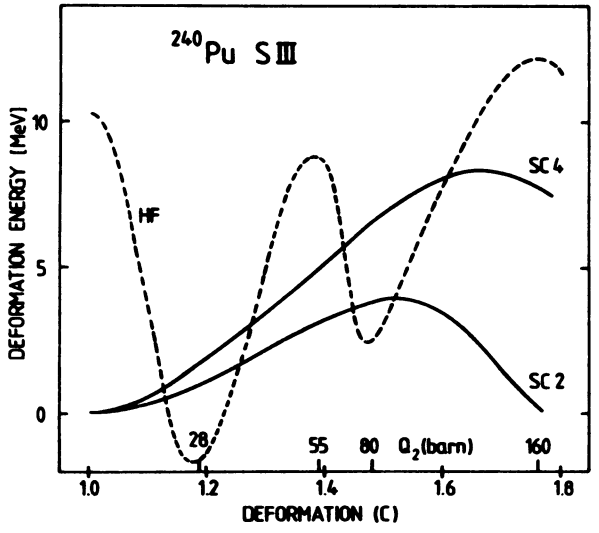

Fig. 3

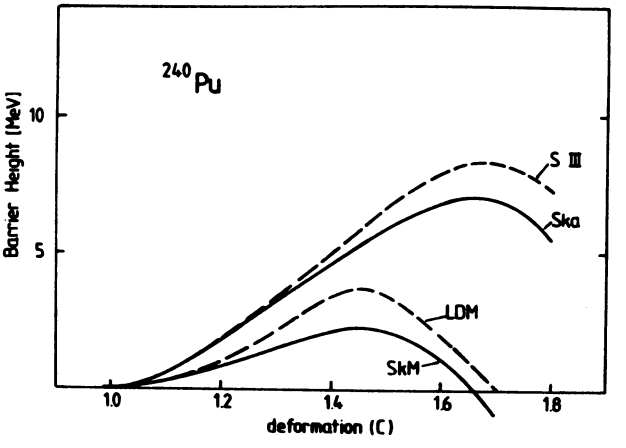

Fig. 4

truncations and spurious energies which are not encountered in the semi-classical calculations.

Anyhow, we see in fig. 4 that there exists a Skyrme force, the SkM force, which leads to an average fission barrier height of about 2.5 MeV, thus lower than the liquid drop [4] value of 3.5 MeV. The location of the saddle point in the {c,h} deformation space is moreover very close to the liquid drop prediction [9] . HF calculations have now been performed for this force [8] and comparisons with our ETF calculation show a nice agreement.

An interesting aspect of the semi-classical approximation, based on the fact that shell fluctuations are smoothed out, is that it permits a direct access to the liquid-drop properties of the effective force under consideration. In the following we shall in a very simple way extract some liquid-drop parameters and check typical relations stated by the droplet model of Myers and Swiatecki [4] . The mass formula we start from has the following form:

$$E = (a_v + JI^2)A + (a_s - \frac{9}{4}\frac{J^2}{Q}I^2)A^{2/3} + (a_c + a_{cs}I^2)A^{1/3}.$$

(For further information on this structure and the parameters for I=0, see the next section).

An important point in most droplet model studies is that the curvature terms are neglected. This is also the case in the newest macroscopic-microscopic computations, which exhibit an extremely good agreement with empirical data, of ground state masses and fission barriers by Möller and Nix [11] with a model in which the mean curvature energy is identically zero. This is at variance with our model using Skyrme forces, as visible in fig. 5 where we have plotted the quantity $(E/A-a_v)A^{1/3}$ against $A^{-1/3}$. The ordinate at origin provides the surface energy, a_s, while the slope measures the curvature energy, a_c, which clearly here is not zero. The surface asymmetry coefficient is

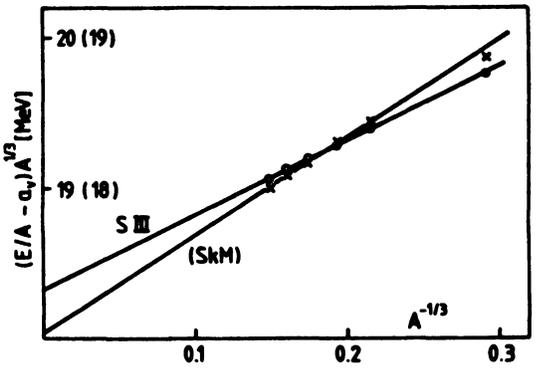

Fig. 5

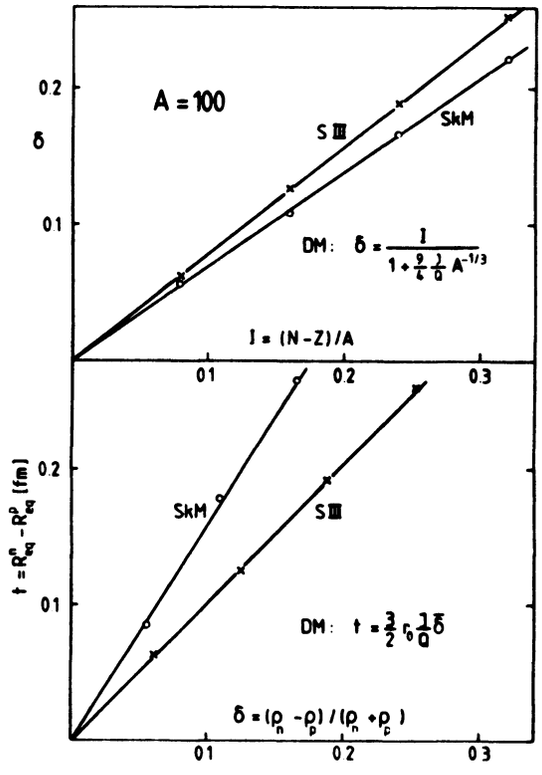

Fig. 6

determined by using the fact that the central density asymmetry $\delta = (\rho_n^\circ - \rho_p^\circ)/(\rho_n^\circ + \rho_p^\circ)$ depends linearly on the isospin I when the total number of nucleons, A, is kept constant. This linear behaviour predicted by the droplet model is also found to be exact in our energy density formalism, see fig. 6. For the sake of clarity the Coulomb interaction is

not included. An alternative way to get the surface asymmetry coefficient is to look at the variation of the neutron skin thickness t(t = $R_n - R_p$, where the radii are the equivalent sharp surface radii) upon the variable δ, which according to the droplet model is also linear, a statement here confirmed. The surface asymmetry coefficient extracted from the slope $dt/d\delta$ is in full agreement with the previous estimate (see fig. 6). Finally the curvature asymmetry coefficient can also be, with a larger uncertainty, deduced from the slope dE/dI^2 for a given A. It is interesting to note

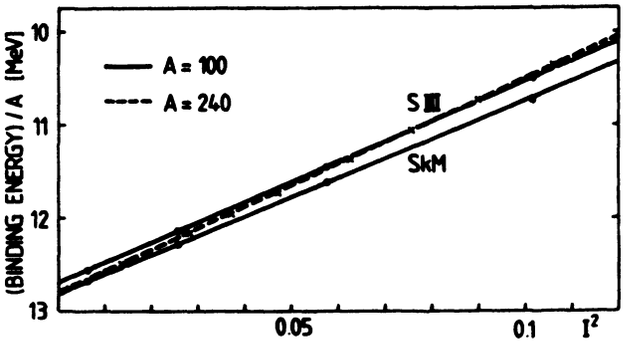

Fig. 7

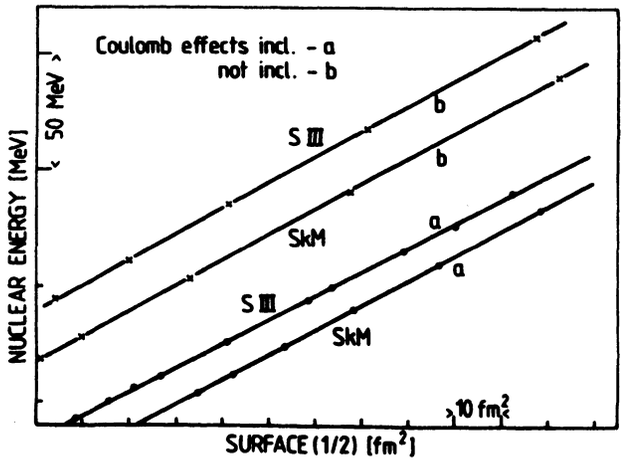

Fig. 8

that the quadratic dependence of E on the isospin is verified even for larger values of I as seen in fig. 7. In table 2 we have written all the coefficients we calculated by these simple methods and compared them to the output of a least squares fit of the function $E(A, I^2)$ to the calculated binding energies of a randomly chosen ensemble of nuclei. Note that the root-mean-square-errors (RMS) for these fits are less than 0.06 MeV. A good agreement between the two methods is observed, thus unambigously showing the strong analogy between the elaborated droplet model and the energy density formalism such as the present ETF model. A systematic analytical derivation of this analogy, restricted so far for symmetric nuclei (I=0), is the object of

the following section. A last observation which will be useful for the following is given in fig. 8 where we show the nuclear part of the total binding energy against the half-density surface. One sees that, at least for changes of surface areas not larger than those occurring up to typical saddle point deformations, the nuclear energy is approximately proportional to the surface. We also checked the selfconsistency effect of the Coulomb energy on the effective surface energy $\frac{dE}{ds}$ and found it to be in fact very small. The omission of the Coulomb energy in the minimization would reduce the effective surface energy by about 0.3 MeV for the SkM force and less than 0.1 MeV for the SIII force. That the nuclear energy is directly proportional to the surface area, seems to contradict our previous claim that curvature energy was non-zero. There is, in fact no contradiction since along the fission path it turns out that the mean curvature of the deformed shape increases approximately linearly with the surface up to the liquid-drop saddle point (see table 5 below).

Force	$k_F^*[fm^{-1}]$	a_v^*[MeV]	J^*[MeV]	a_s[MeV]	Q[MeV]	a_c[MeV]	a_{cs}[MeV]
SIII	1.29	-15.86	28.16	18.30 18.3	49.4 50	4.87 5.0	23.4 21.3
SkM	1.33	-15.78	30.75	17.18 17.2	38.9 35.5	6.09 6.4	23.7 36.5

Table 2. Droplet model parameters of the forces SIII and SkM.

* calculated for infinite nuclear matter

the lower values are from the droplet relations (see text)

III. Leptodermous expansion of the total energy of symmetric nuclei

a. Intrinsic nuclear shape coordinate system

The experimental fact that the nuclear surface diffusivity is nearly independent of the nucleon number and thus of the curvature allows to approximate the nucleon densities to be functions essentially only of a coordinate along the normal direction to the equivalent sharp liquid drop surface, once its deformation has been fixed. It is thus natural to introduce a system of curvilinear coordinates such that two of the coordinates describe the sharp surface for each given shape of the nucleus, while the third measures the distance from the surface. Such a coordinate system has been introduced in ref. [12]; for completeness we recall here its main features.

Restricting ourselves to axially symmetric nuclear shapes, we start from cylindrical coordinates (ρ, z', φ) in which the nuclear sharp surface is described by a function $\rho = f(z')$ (see Fig. 9). From any point $P(\rho, z')$ we go over to the coordinates (u,z) defined for each given shape function $f(z')$ by

$$\begin{aligned} z' &= z + u\cos\alpha \quad , \quad \cos\alpha = -\frac{f'(z)}{\sigma(z)} \; ; \\ \rho &= f(z) + u\sin\alpha \quad , \quad \sin\alpha = 1/\sigma(z) \; ; \end{aligned} \tag{1}$$

with

$$\sigma(z) = \sqrt{1 + [f'(z)]^2} \; . \tag{2}$$

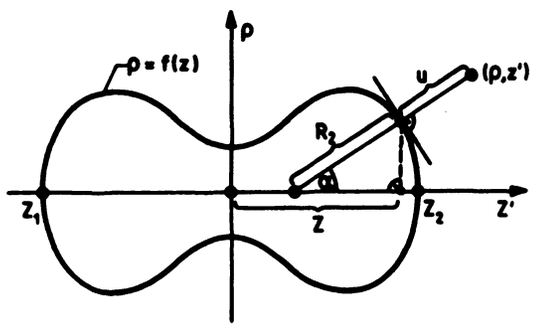

Fig. 9

Thus, as illustrated in Fig. 9, the new coordinate u is the distance of $P(\varphi, z')$ perpendicular to the surface (taken to be positive outside and negative inside), whereas z is the z' coordinate of the projection of $P(\rho, z')$ onto the surface along the normal. The system of curvilinear coordinates (u, z, φ) is orthogonal. Calculating the Jacobian of the above transformation, one finds that the volume element is given by

$$d^3r = \rho\, d\rho\, dz'\, d\varphi = g(u,z)\, du\, dz\, d\varphi , \tag{3}$$

where

$$g(u,z) = \left(1 + \frac{u}{R_1}\right)(u + R_2) \tag{4}$$

and R_1, R_2 are the main curvature radii given in terms of f(z) and $\sigma(z)$ eq. (2) by

$$R_1^{-1} = - \frac{f''(z)}{[\sigma(z)]^3} , \qquad R_2 = \sigma(z) f(z) . \tag{5}$$

The range of the variable z is $z_1 \leq z \leq z_2$ and that of u is $-R_2 \leq u < \infty$. Thus the volume V_0 inside the surface described by $\rho = f(z)$ (i.e. $u = 0$) is

$$V = 2\pi \int_{z_1}^{z_2} dz \int_{-R_2}^{0} g(u,z)\, du \equiv \pi \int_{z_1}^{z_2} f^2(z)\, dz . \tag{6}$$

The surface area is given by

$$S = \int dS = 2\pi \int_{z_1}^{z_2} \sigma(z) f(z)\, dz = 2\pi \int_{z_1}^{z_2} R_2\, dz . \tag{7}$$

For the following it is also interesting to define the mean curvature H and the Gaussian curvature G:

$$H = \frac{1}{2}(R_1^{-1} + R_2^{-1}) \quad , \quad G = (R_1 R_2)^{-1} . \tag{8}$$

The surface integral of H, which we in the following just call the "mean curvature" C, is

$$C = 2\pi \int_{z_1}^{z_2} H R_2 \, dz = \pi \int_{z_1}^{z_2} \left(1 + \frac{R_2}{R_1}\right) dz . \tag{9}$$

The surface integral over G is constant :

$$2\pi \int_{z_1}^{z_2} R_2 \, G \, dz = 2\pi \int_{z_1}^{z_2} \frac{1}{R_1} \, dz = 4\pi \tag{10}$$

as a special case of the Gauss-Bonné law. Eq. (10), which holds for any connected smooth shape, can easily be proven by substituting $x = f'(z)$ and integrating over x. For separated shapes (after scission), the value will of course be 8π.

Our approximation to the semiclassical nucleon densities is that they only depend on the variable u. As found in the variational calculations of refs. [1,3], Fermi functions minimize rather well the semiclassical Skyrme energy in the spherical case. We thus parametrize the densities as follows

$$\left.\begin{aligned} \rho_n(\vec{r}) = \rho_n(u) &= \frac{\rho_{n0}}{1 + \exp\left(\frac{u+\Delta}{a_n}\right)} \\ \rho_p(\vec{r}) = \rho_p(u) &= \frac{\rho_{p0}}{1 + \exp\left(\frac{u-\Delta}{a_p}\right)} . \end{aligned}\right\} \tag{11}$$

Thus, we allow the protons and neutrons to have different (but "parallel") surfaces with a radius difference 2Δ. This leaves us, together with an overall scale parameter (e.g. $2c = z_2 - z_1$), with 6 parameters, two of which are eliminated by the particle number conservation

$$\int d^3r\, \varrho_n(\vec{r}) = N\,, \quad \int d^3r\, \varrho_p(\vec{r}) = Z\,. \tag{12}$$

The other 4 parameters are determined variationally by minimizing the total energy

$$\delta \int d^3r\, \mathcal{E}[\varrho_n, \varrho_p] = 0 \tag{13}$$

with the subsidiary conditions eq. (12). In calculating the Skyrme energy density $\varepsilon[\rho_n, \rho_p]$ with the semiclassical kinetic energy density functionals $\tau[\rho]$ and $\vec{J}[\rho]$ (see refs. [6,13]), we need also the first and second derivatives of $\rho_q(\vec{r})$. In the present coordinates, one obtains simply

$$|\nabla \varrho|^2 = [\varrho'(u)]^2\,, \tag{14}$$

$$\Delta \varrho(u) = \varrho''(u) + \left[\frac{1}{u+R_1} + \frac{1}{u+R_2}\right] \varrho'(u)\,.$$

b. Leptodermous expansion of the energy for symmetrical nuclei

We now proceed to calculate the total energy for symmetric nuclei (with $\rho_n = \rho_p = \frac{1}{2}\rho$):

$$E = \int d^3r\, \mathcal{E}(\varrho) = 2\pi \int_{z_1}^{z_2} dz \int_{-R_2}^{\infty} g(u,z)\, \mathcal{E}[\varrho(u)]\, du \tag{15}$$

in the "leptodermous" approximation, i.e. in the limit where the curvature R_2 is everywhere large compared to the surface diffusivity $\alpha = \alpha_p = \alpha_n$:

$$R_2 \gg \alpha \ . \tag{16}$$

This approximation should be well fulfilled for heavy nuclei up to typical saddle point deformations which for actinide nuclei have almost no neck. In the limit (16), the lower limit of the u-integration in eq. (15) (which, in fact, is the only reason for the integral not to separate in u and z!) can be practically replaced by $-\infty$ for all contributions except the one which gives the volume energy. We therefore separate the latter out in writing

$$E = a_v A + \Delta E, \quad a_v = \mathcal{E}[\rho_0]/\rho_0 , \tag{17}$$

where ρ_0 is the density at the centre. The correction E is then

$$\Delta E = 2\pi \int_{z_1}^{z_2} dz \int_{-R_2}^{\infty} du \, g(u,z) \left\{ \mathcal{E}[\rho] - a_v \rho(u) \right\} . \tag{18}$$

The leptodermous approximation (to be checked numerically below) thus consists in writing ΔE, which contains only contributions near the surface, i.e. in a region $-\alpha \lesssim u \lesssim +\alpha$, as

$$\Delta E \approx 2\pi \int_{z_1}^{z_2} dz \int_{-\infty}^{+\infty} du \, g(u,z) \left\{ \mathcal{E}[\rho] - a_v \rho(u) \right\} . \tag{19}$$

Since the integral now separates, we obtain with eqs. (4, 7, 9, 10)

$$\Delta E \approx b_0 \cdot S + b_1 \cdot 2C + b_2 \cdot 4\pi , \tag{20}$$

where the coefficients b_0, b_1 and b_2 can be obtained once for all for a given energy density as functions of ρ_0, α and the force parameters and do not depend on deformation and nucleon number A. The main A dependence (except a very weak one through ρ_0 and α) and the entire deformation dependence are contained in S and C.

The explicit expressions for the coefficients b_n are given in the following. Because of the explicit z dependence (through R_1, R_2) of the Laplacian $\Delta\rho$ (see eq. 14) we have to split up the total energy density. Writing

$$\mathcal{E}[\rho] = \mathcal{F}(u) + \mathcal{G}(u)\Delta\rho + \mathcal{H}(u)[\Delta\rho]^2, \tag{21}$$

where the functions $\mathcal{F}$, $\mathcal{G}$ and $\mathcal{H}$ may only depend on ρ and $\nabla\rho$, one gets

$$\begin{aligned}
b_0 &= \int_{-\infty}^{+\infty} \{\mathcal{F}(u) + \mathcal{G}(u)\rho''(u) + \mathcal{H}(u)[\rho''(u)]^2 - a_v\rho(u)\}\, du , \\
b_1 &= \int_{-\infty}^{+\infty} \{u\mathcal{F}(u) + \mathcal{G}(u)\rho'(u) + 2\mathcal{H}(u)\rho'(u)\rho''(u) - u a_v\rho(u)\}\, du , \\
b_2 &= \int_{-\infty}^{+\infty} \{u^2\mathcal{F}(u) + 2u\rho'(u)[\mathcal{G}(u) + 2\mathcal{H}(u)\rho''(u)] + 4\mathcal{H}(u)[\rho'(u)]^2 \\
&\qquad - u^2 a_v\rho(u)\}\, du .
\end{aligned} \tag{22}$$

In eqs. (22), the primes on ρ denote derivation with respect to u. In arriving at this result, we have neglected a term

$$2\pi \int_{z_1}^{z_2} dz \frac{1}{R_1} \int_{-R_2}^{\infty} du\, \mathcal{H}(u) [\rho'(u)]^2 \left(\frac{R_1 - R_2}{u + R_2} + \frac{R_2 - R_1}{u + R_1} \right) \tag{23}$$

whose deformation dependence is more complicated than that of the above simple invariants C,S or a constant. However, this term is seen to be exactly zero in the spherical case and negligibly small otherwise.

In order to sort out the deformation and nucleon number (A) dependence of S and C, we must now impose the conservation of A. In the leptodermous expansion we get

$$A = \int d^3r\, \rho(\vec{r}) = V + \frac{\pi^2}{3} \alpha^2 C + O\left[e^{-R_2/\alpha}\right] \tag{24}$$

The contributions of order $\exp(-R_2/\alpha)$ are practically negligible for not too light nuclei ($A \gtrsim 20$). In the spherical case we have $V = (4\pi/3)R_{1/2}^3$, $S = 4\pi R_{1/2}^2$ and $C = 4\pi R_{1/2}$, where $R_{1/2}$ is the "sharp" or half density radius which is adjusted to keep A constant. For the deformed case we introduce in the usual manner the shape functions B_S and B_C, which are normalized to unity for the spherical case, by defining

$$S = 4\pi R_{1/2}^2 B_S \quad , \qquad C = 4\pi R_{1/2} B_C \, . \tag{25}$$

With that we get

$$A \approx \frac{4\pi}{3} \rho_0 \left[R_{1/2}^3 + \pi^2 \alpha^2 R_{1/2} B_C \right] , \tag{26}$$

from where we find in a very good approximation

$$R_{1/2} \approx r_0 A^{1/3} - \frac{\pi^2 \alpha^2}{3 r_0} A^{-1/3} B_C \, . \tag{27}$$

Here the radius r_0 is defined by $r_0 = (3/4\pi\rho_0)^{1/3}$.

We now can insert $R_{1/2}$ eq.(27) into eqs.(25) and arrive with eqs.(17,20) at the leptodermous expansion of the total energy:

$$E = a_v A + a_s A^{2/3} + a_c A^{1/3} + a_0 + O(A^{-1/3}), \qquad (28)$$

where

$$a_s = 4\pi r_0^2 B_s b_0 \qquad (29)$$

$$a_c = 8\pi r_0 B_c b_1 \qquad (30)$$

$$a_0 = 4\pi b_2 - \frac{6}{3}\pi^3 \alpha^2 B_s B_c b_0 \qquad (31)$$

The terms of order $A^{-1/3}$ and lower contribute less than 1 MeV to the total energy of heavy nuclei and are thus practically unimportant. The deformation dependence of the energy (28) is entirely contained in the shape functions B_s and B_c. The main A dependence of the energy is also separated out in eq.(28); a very smooth variation is, however, still coming from the b_n and r_0 through their dependence on ρ_0 and α which are determined for each nucleus by the variational equation (13).

c. Dependence of the central density ρ_0 on the nucleon number A

The deviation of the central density ρ_0 of finite nuclei from the saturation density ρ_∞ of infinite nuclear matter has traditionally been estimated from the saturation condition itself [4,12]. The latter is automatically fulfilled if we write the energy density of infinite nuclear matter in the form [+)]

+) This form implies that $(\rho_\infty)^2 \mathcal{E}''_\infty(\rho_\infty) = \frac{1}{3} K_\infty$ which is found to be fulfilled within ~ 5 % for the Skyrme force dicussed in the next section.

$$\mathcal{E}_\infty(\rho) = \rho\left[a_v^\infty + \frac{1}{18} K_\infty \left(\frac{\rho-\rho_\infty}{\rho_\infty}\right)^2\right]. \tag{32}$$

Here K_∞ is the nuclear incompressibility defined by

$$K_\infty = 9(\rho_\infty)^2 \frac{d^2}{d\rho^2}\left[\frac{\mathcal{E}_\infty(\rho)}{\rho}\right]_{\rho=\rho_\infty}. \tag{33}$$

For a given Skyrme force a_v^∞, ρ_∞ and K_∞ are uniquely given constants. Now, the variational equation for a finite symmetric nucleus (without Coulomb force), viz.

$$\delta \int d^3r \left\{ \mathcal{E}[\rho] - \lambda\rho(\vec{r}) \right\} = 0, \tag{34}$$

with the Lagrange multiplier λ for nucleon number conservation, can be solved easily at the centre of the nucleus using the functional $\mathcal{E}_\infty(\rho)$ eq. (32), if the surface contributions are all exponentially small there. Then, the only parameter to be varied is ρ_0, and eq. (34) takes the form

$$a_v^\infty - \lambda - \frac{K_\infty}{3}\epsilon + \frac{3}{2}K_\infty\epsilon^2 = 0\,; \qquad \epsilon = -\frac{1}{3}\frac{(\rho_0-\rho_\infty)}{\rho_\infty}. \tag{35}$$

The A dependence thus comes in only through the Fermi energy λ. The latter is found from eq. (28) with $\lambda = dE/dA$. To lowest order in $A^{-1/3}$ one obtains

$$\epsilon_0 = -\frac{2}{K_\infty} a_s^\infty A^{-1/3}, \tag{36}$$

which is the usual droplet model result [4]. Expanding the coefficients a_v and a_s around the saturation density ρ_∞:

$$a_v(\rho_0) = a_v^\infty + \frac{K_\infty}{2}\epsilon^2 \quad , \quad a_s(\rho_0) = a_s^\infty - 3\rho_\infty a_s'(\rho_\infty)\epsilon \, , \tag{37}$$

one gets up to order $A^{-2/3}$

$$\epsilon = \frac{1}{9} - \frac{1}{9}\sqrt{1 + \frac{36}{K_\infty}\left(a_s^\infty A^{-1/3} + \frac{1}{2}a_c^* A^{-2/3}\right)} \tag{38}$$

with

$$a_c^* = a_c^\infty + \frac{2}{K_\infty}a_s^\infty\left[a_s^\infty + 3\rho_\infty a_s'(\rho_\infty)\right] . \tag{39}$$

As we will show in the next section, eq. (38) does not reproduce very well the central density ρ_0 found numerically with the energy density method. The reason for this is not the inadequacy of the leptodermous expansion as such, but the fact that the Fermi type densities used above (and in the droplet model) are not exactly solutions of the Euler equations (13). Thus, the local variation at the centre, eq. (35), does not lead to the same result as the global variation, eq. (13), of the total energy with respect to the parameters of the Fermi function.

It is therefore more consistent to derive the central density ρ_0 from the variation of the total energy as obtained in the leptodermous expansion in eq. (28). Neglecting the α dependence (which is very weak, as shown in sect. e below), we thus write

$$\frac{dE}{d\rho_\infty} = A\frac{da_v}{d\rho_\infty} + A^{2/3}\frac{da_s}{d\rho_\infty} + \ldots = 0 . \tag{40}$$

Using eq. (37) we get to order $A^{-1/3}$

$$\epsilon_0 = \frac{3}{K_\infty}\rho_\infty a_s'(\rho_\infty) A^{-1/3} . \tag{41}$$

If the density profile is chosen such as to maximize exactly the parameter b_0 eq. (22) (which is equal to the surface tension for semi-infinite nuclear matter), then the rate of change of the surface energy with respect to ρ_0 would be equal to [4]

$$\rho_\infty a_s'(\rho_\infty) = -\frac{2}{3} a_s^\infty \tag{42}$$

and the two solutions of ϵ_0, eqs. (41) and (36) would be identical. This is however not the case, neither if the Euler equation of finite nuclei is exactly solved, nor if one fixes the density to a Fermi function. In the case considered numerically below, the difference between the two sides of eq. (42) is ~10 % (for other interactions it may even be larger).

A more accurate result for ϵ, valid also for lighter nuclei, is obtained by expanding further up to terms of order $A^{-2/3}$:

$$\epsilon = \frac{\rho_\infty\left[a_s'(\rho_\infty)A^{-1/3} + a_c'(\rho_\infty)A^{-2/3}\right]}{3\left\{\frac{K_\infty}{9} + \rho_\infty^2\left[a_s''(\rho_\infty)A^{-1/3} + a_c''(\rho_\infty)A^{-2/3}\right]\right\}} . \tag{43}$$

With eq. (43), the central densities found numerically are reproduced within less than $10^{-3}\rho_0$ for $A \gtrsim 100$, thus demonstrating the validity of the leptodermous expansion.

d. Incompressibilty of finite nuclei

Based on these results, it is now easy to derive an expression for the incompressibilty of finite nuclei, defined by

$$K_A = 9\,\rho_0^2\,\frac{d^2}{d\rho_0^2}\left(\frac{E}{A}\right) \tag{43.a}$$

(see, e.g. ref. [16]). Analogously to eq. (40) we derive the parameters a_V, a_S, ... to obtain

$$K_A = \left(\frac{\rho_0}{\rho_\infty}\right)^2\left[K_\infty - 27\rho_\infty^3 a_V''' \epsilon + 9\rho_\infty^2\left(a_S'' A^{-1/3} + a_C'' A^{-2/3}\right) + \ldots\right]. \tag{43.b}$$

In expanding K_A eq. (43.b) consistently up to order $A^{-1/3}$, one should also respect the first factor on the r.h.s., which is equal to $(1-3\epsilon)^2$ (and which was omitted in ref. [16]), leading to

$$K_A = K_\infty + 9\left[\rho_\infty^2 a_S'' - 2\rho_\infty a_S' - \frac{9}{K_\infty}\rho_\infty^4 a_S' a_V'''\right]A^{-1/3} + O\left(A^{-2/3}\right). \tag{43.c}$$

(Here the derivatives a_S', a_S'', etc. are taken at ρ_∞, as above.) Again, we will see in the next section that this expression agrees very well with the numerical results for K_A eq. (43.a).

e. Numerical tests of the leptodermous approximation

Before presenting some quantitative tests of the quality of the leptodermous approximation, we shall write down some explicit expressions using the traditional parametrization of Skyrme forces, restricting ourselves hereby to symmetric nuclei without Coulomb interaction. The energy density then has the explicit form [14]

$$\mathcal{E}[\rho] = \frac{\hbar^2}{2m}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^3 + \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 + \frac{1}{16}(3t_1 + 5t_2)\tau\rho + \frac{3}{4}W_0\,\vec{\nabla}\rho\cdot\vec{J}. \quad (44)$$

The semiclassical functionals $\tau[\rho]$ and $\vec{J}[\rho]$ are given in refs. [6,13] Under the integral eq. (15), the expression for $\mathcal{E}[\rho]$ can be simplified using partial integrations so that only powers of $\vec{\nabla}\rho$ and $\Delta\rho$ are needed. For the sake of simplicity, we give here only the results including the second order contributions $\tau_2[\rho]$ and $\vec{J}_2[\rho]$ of the semiclassical functionals. The energy density $\mathcal{E}[\rho]$ then takes the simple form [3]

$$\mathcal{E}[\rho] = \varkappa\rho^{5/3}(1+\beta\rho) + e\rho^2 + f\rho^3 + \sigma(\nabla\rho)^2 + \eta\frac{(\nabla\rho)^2}{\rho} - \zeta\rho\frac{(\nabla\rho)^2}{(1+\beta\rho)} \quad (45)$$

with the constants defined by

$$\varkappa = \frac{\hbar^2}{2m}\cdot\frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}, \quad e = \frac{3}{8}t_0, \quad f = \frac{1}{16}t_3, \quad \eta = \frac{1}{36}\frac{\hbar^2}{2m},$$

$$\beta = \frac{2m}{\hbar^2}\cdot\frac{1}{16}(3t_1 + 5t_2), \quad \zeta = \frac{1}{12}\cdot\frac{\hbar^2}{2m}\beta^2 + \frac{m}{\hbar^2}\left(\frac{3}{4}W_0\right)^2,$$

$$\sigma = \frac{1}{64}(9t_1 - 5t_2) - \frac{11}{36}\frac{\hbar^2}{2m}\beta = \frac{1}{12}\left(t_1 - \frac{25}{12}t_2\right). \quad (46)$$

The integrals entering the definition of the surface tension b_0 eq. (22) can all be done analytically [6]. This is no longer so for some contributions to the parameters b_1 and b_2 in eq. (22). However, for a force with constant effective nucleon mass $m^* = m$ (i.e. if $\beta = 0$), all the leptodermous integrals in eq. (22) can be done once for all and their explicit dependence on the density parameters ρ_0 and α is known. Such a force has been published with the label S VII [15]; its parameters are given in Table 3

of α, less than 1 % over the range considered here, is so weak for the present case that we may replace it by the value $\alpha_\infty = 0.412$ (obtained by minimizing the surface tension b_o at $\rho_o = \rho_\infty$, which easily is done analytically), without affecting the total energies by more than ~ 0.5 MeV. Then, the determination of ρ_o can be done as described in sect. C above; the result quoted

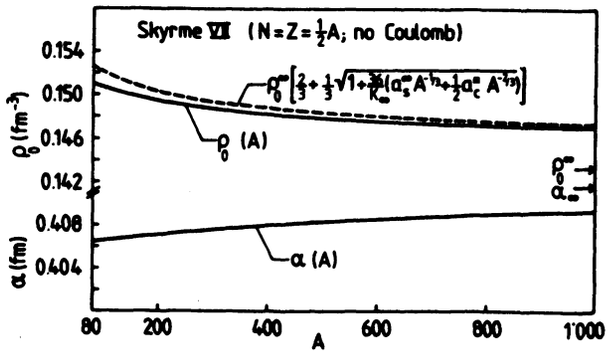

Fig. 10

in eq. (43) then still reproduces the exact numerical values $\rho_o(A)$ in fig. 10 within ~ 1 °/oo for A > 100. The dashed line in the figure shows the central density obtained by applying the variational equation locally at the centre of the nucleus. As we stated in sect. C, the discrepancy comes here mainly from the difference between the leading term of eq. (43) and the traditional droplet model value eq. (36) of the quantity ϵ_∞.

The values of the leptodermous integrals eq. (22), taken at $\rho_o = \rho_\infty$, are

$$b_o = 0.9972 \text{ MeV fm}^{-2}, \quad b_1 = 0.3347 \text{ MeV fm}^{-1}, \quad b_2 = 0.6692 \text{ MeV}. \tag{50}$$

From them and their variations with ρ_o we find (all quantities in MeV):

$$\begin{aligned}
a_s^\infty &= 17.61, & \rho_\infty a_s'(\rho_\infty) &= -10.8, & \rho_\infty^2 a_s''(\rho_\infty) &= -84.6; \\
a_c^\infty &= 9.97, & \rho_\infty a_c'(\rho_\infty) &= 22.0, & \rho_\infty^2 a_c''(\rho_\infty) &= 39.4; \\
a_o^\infty &= -5.65, & \rho_\infty a_o'(\rho_\infty) &= -1.1, & \rho_\infty^2 a_o''(\rho_\infty) &= 39.2.
\end{aligned} \tag{51}$$

Table 3

Parameters and infinite nuclear matter properties of the Skyrme SVII force [15].

t_0 (MeV fm^3)	t_1	t_2	W_0 (MeV fm^5)	t_3 (MeV fm^6)	x_0	x_1	x_2	x_3
- 1096.8	246.3	-147.8	112.0	17 626.0	0.62	0	0	1.0

ρ_∞ (fm^{-3})	r_0^∞ (fm)	K_∞ (MeV)	a_v^∞ (MeV)
0.14332	1.1854	366.23	-15.782

along with the corresponding infinite nuclear matter properties. The results of the integrals in eq. (22) are then

$$b_0 = \alpha\left[\overbrace{-0.7590\,\varkappa\rho_0^{5/3} - e\rho_0^2 - \tfrac{3}{2}f\rho_0^3}^{A}\right] + \frac{1}{\alpha}\left[\overbrace{\tfrac{1}{6}\sigma\rho_0^2 + \tfrac{1}{2}\eta\rho_0 - \tfrac{1}{12}\zeta\rho_0^3}^{B}\right], \quad (47)$$

$$b_1 = \alpha^2\left[-0.1275\,\varkappa\rho_0^{5/3} + \tfrac{1}{2}f\rho_0^3\right] + \tfrac{1}{2}\eta\rho_0 + \frac{1}{48}\zeta\rho_0^3, \quad (48)$$

$$b_2 = \alpha^3\left[-2.6016\,\varkappa\rho_0^{5/3} - 3.2899\,e\rho_0^2 - 4.9348\,f\rho_0^3\right] + \quad (49)$$
$$+ \alpha\left[0.2150\,\sigma\rho_0^2 + 1.6449\,\eta\rho_0 - 0.3225\,\zeta\rho_0^3\right].$$

(The expression for b_0 is consistent with the result given in ref. [6].)
It is now an easy matter to calculate the energy according to eqs. (28)-(31) and to minimize it with respect to ρ_0 and α.

Fig. 10 shows the resulting values obtained for spherical nuclei with the Skyrme force S VII as functions of the mass number A [+]. The variation

[+] Here, as in the following, all 4. order contributions to the semiclassical functionals $\tau[\rho]$ and $\vec{J}[\rho]$ have been included.

With that, the leptodermous expansion of the total energy eq. (28), after expanding out the A dependence using eq. (43), becomes

$$E = a_v^{\infty} A + a_s^{\infty} A^{2/3} + a_c^{*} A^{1/3} + a_o^{*} \quad . \tag{52}$$

The expression for a_c^* has already been given in eq. (39). The quantity a_o^* receives many contributions from expanding a_v, a_s and a_c around ρ_∞; its expression in terms of the quantities in eq. (51) is straightforward but cumbersome and has not much practical value, since the parameter a_o^* can not be determined reasonably well in any least-squares fit, as we shall see below.

σ	a_v^{∞}	a_s^{∞}	a_c^*	a_o^*	a_{-1}	a_{-2}
leptod.	- 15.782	17.61	8.53	- 2.74	-	-
0.004	- 15.789	17.56	8.57	- 10.01	4.6	8.7
0.06	- 15.778	17.34	9.81	- 10.81	0[a]	0[a]
3.45	- 15.782[a]	17.61[a]	8.53[a]	- 16.24	0[a]	0[a]
0.51	- 15.782[a]	17.61[a]	6.40	0.47	0[a]	0[a]
0.30	- 15.782[b]	17.61[b]	6.17	2.48	0[b]	0[b]

Table 4 Liquid drop parameters of the expansion eq. (52) of the total energy obtained in the exact variational calculation for symmetric nuclei with the force S VII (no Coulomb).

(All results in MeV). The first line gives the parameters obtained in the leptodermous expansion. The others give the results of different least-squares fits to the exact results for 24 nuclei ranging from A=80 to A=1000 (except in the last line for only 21 nuclei with $200 \leqslant A \leqslant 1000$). σ is the root mean square deviation in MeV. a_{-1} and a_{-2} are the coefficients of terms proportional to $A^{-1/3}$ and $A^{-2/3}$, respectively.

a) value fixed in the fitting to 24 nuclei.

b) value fixed in the fitting to 21 nuclei.

In Table 4 we list the 4 parameters of eq. (52) obtained in the leptodermous approximation along with the results of several least-squares fits to the total exact energies (obtained numerically from the variational calculation without any further approximation). We see that, apart from the ambiguities of such fits themselves (especially concerning the constant term a_o^*!), there is an excellent agreement. This shows, that one is in principle able to determine sufficiently accurately the three leading terms of the expansion (52) for a given Skyrme force just in terms of the simple 1-dimensional integrals eq. (22). (Which, of course, can be done also for a realistic force including a variable effective mass.)

To test the validity of the leptodermous expansion as a function of the deformation, we have made a calculation for A = 240 using the shape parametrization (c, h) used in connection with fission barrier calculations [9]. In Table 5 we present various quantities as a function of the elongation parameter c (h = 0). The spherical shape corresponds to c=1, the liquid drop

c	neck radius (fm)	B_s	B_c	$R_{1/2(fm)}$	$R^{lept.}_{1/2}$ (fm)	$E - a_v A$ (MeV)	$\Delta E_{lept.}$ (MeV)	error (MeV)
1.0	7.19	1.0	1.0	7.1935	7.1939	712.3	722.1	9.8
1.2	6.45	1.0151	1.0168	7.1922	7.1927	723.0	733.0	10.0
1.4	5.73	1.0546	1.0654	7.1885	7.1890	751.7	761.7	10.0
1.6	4.93	1.1146	1.1486	7.1822	7.1828	796.0	806.1	10.1
1.8	3.90	1.1925	1.2750	7.1725	7.1733	854.5	865.0	10.5
2.0	2.26	1.2745	1.4730	7.1576	7.1586	920.0	931.1	11.1

Table 5

Various quantities obtained for A = 240 with force Skyrme SVII versus elongation c (see text for details).

saddle point of actinide nuclei to c ≃ 1.5. The second column shows the neck radius of the corresponding shape which is strongly constricted at c = 2.0. The next three columns contain the shape functions B_s and B_c and the radius scaling parameter $R_{1/2}$, from which the surface area S and the mean curvature C are obtained via eqs. (25). It is worth noting that, with the values $\rho_o = 0.1492$ fm^{-3}, $\alpha = 0.408$ fm valid for A = 240, the leptodermous result $R_{1/2}^{lept}$ eq. (27), shown in the next column, reproduces the exact values within $\sim 10^{-4} R_{1/2}$ even at the largest deformation. In columns 7 and 8 of table 5 we show the total energy minus the volume energy and the leptodermous result eq. (20) for ΔE, respectively; their difference is shown in the last column. Apart from a constant error of ~ 10 MeV, which reflects the difficulties in determining the constant term of the energy expansion eq. (52) observed above, there is only a small variation of $\lesssim 1.3$ MeV over the whole range of deformation. This is rather astonishing, observing the small neck radius of 2.26 fm at the largest deformation. Up to typical saddle point deformations ($c < 1.6$), the error in the deformation energy brought about by the leptodermous expansion is even not larger than 0.3 MeV.

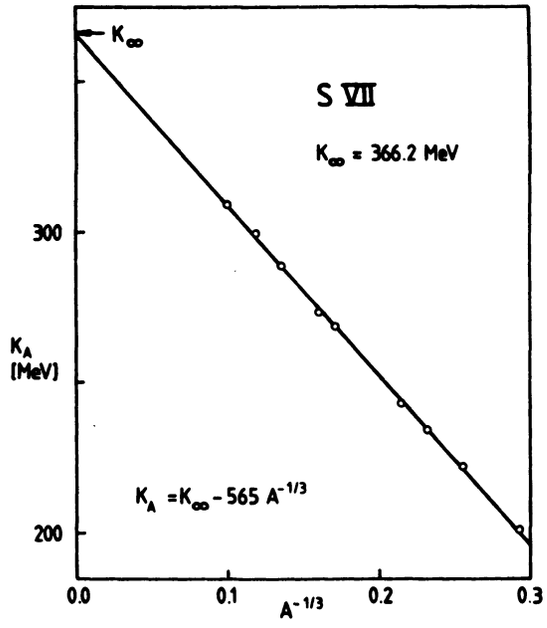

Fig. 11

In order to test finally the expression given above for the incompressibility of finite nuclei K_A, eq. (43.c), we present in Fig. 11 the numerical results of K_A according to eq. (43.a) with the SVII force. The behaviour of K_A versus $A^{-1/3}$ is linear, showing that the $A^{-2/3}$ term in eq. (43.c) is very small. The results of Fig. 11 give

$$K_A = K_\infty - A^{-1/3} \times 565 \text{ MeV}. \tag{53}$$

With the values in eq. (51) and with $\rho_\infty^3 a_v^{WI} = 5.8$ MeV for SVII we obtain for the leptodermous expansion eq. (43.c)

$$K_A = K_\infty - A^{-1/3} \times 553 \text{ MeV} - A^{-2/3} \times 6 \text{ MeV}. \tag{54}$$

Thus, the coefficient of $A^{-2/3}$ is, indeed, two orders of magnitude smaller than that of $A^{-1/3}$, which is in excellent agreement with the exact result of eq. (53).

f. Conclusions and outlook

Using the leptodermous expansion, we have demonstrated that the energy density formalism using Skyrme forces allows a quantitative determination of the droplet model type parameters for symmetric nuclei. For asymmetric nuclei including the Coulomb interaction, the analysis becomes more cumbersome, since different density parameters $R_{1/2}$, ρ_0, α have to be used for protons and neutrons. Recent results have shown that the difference in the diffuseness parameters $\alpha_n - \alpha_p$ is clearly correlated to the isospin (N-Z)/A of the nucleus [1], which is an effect not included in the droplet model [4]. Apart from that, the essential droplet model relations for the asymmetry parameters, in particular the effective surface stiffness Q, seem to be fulfilled at least qualitatively. A detailed analysis of the leptodermous expansion in the asymmetric case is presently under way.

Concerning the deformation dependence of the total energy obtained in the semiclassical energy density method, the leptodermous expansion has been shown here to be very accurate even beyond typical saddle point deformations of heavy nuclei. A numerical test of the corresponding expansion of the Coulomb energy is actually under way; if it holds equally well we may conclude that a full variational calculation is not needed in the deformed case. Instead, it would be sufficient to calculate the droplet model parameters for a given force on one hand and the shape functions B_s, B_c and B_{concl} on the other hand once for all and then use eq. (20) (including the Coulomb energy) to obtain the deformation energy. Work along these lines is now in progress.

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