# NUCLEAR CURVATURE ENERGY FROM THRESHOLD ENERGIES

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Abstract: Theoretical studies in the shell model have led to the conclusion that the shape dependence of the liquid-drop part of the semi-empirical mass formula of the Weizsäcker-Bethe type should contain terms proportional to the volume, the surface, and the mean-total curvature of the surface of the drop, respectively. Now the surface tension  $\beta_e$  and the curvature tension  $\gamma_e$  are fitted to the experimentally known fission barriers of 35 nuclei. Furthermore, the parameters of the liquid-drop part of the mass formula are roughly fitted to the ground-state masses of about 600 beta-stable nuclei. For the elementary radius  $r_e$ , the value 1.123 fm (determined by Elton) is used. As a result,  $\gamma_e$  should be in the range 6-8 MeV, with the value 6.8 MeV being the most probable, thus  $\beta_e = 17.85$  MeV. For sufficiently large values of the curvature tension (e.g.  $\gamma_e = 13.4$  MeV), a small double-hump fission barrier occurs in the region of Ra.

## 1. The semi-empirical mass formula

Since Weizsäcker <sup>1</sup>), Bethe and Bacher <sup>2</sup>) proposed their semi-empirical charged liquid-drop formula, which describes fairly accurately the binding energy of nuclei, many calculations have been performed by fitting formulae to the about 1000 experimentally determined ground-state energies of beta-stable nuclei. A summary was given by Wing <sup>3</sup>). Thus the dependence of the nuclear masses M on  $\Delta$  (the atomic weight) is fairly well known. Also the dependence of M on the shape of the nucleus has been considered. Myers and Swiatecki <sup>4,5</sup>) among others suggested a mass formula which, while depending on the deformation of nuclei, includes an effective three-parameter shell-correction term  $E_{\rm shell}$  in addition to the commonly used charged liquid-drop part <sup>†††</sup>  $E_{\rm LD}$  and the pairing energy  $E_{\rm pair}$ , hence

$$M(A, B, \mathscr{C}) = M_{\rm n} N + M_{\rm H} Z + E_{\rm LD}(A, B, \mathscr{C}) + E_{\rm pair}(A, B, \mathscr{C}) + E_{\rm shell}(A, B, \mathscr{C}), \quad (1)$$

where  $M_n$  and  $M_H$  are the neutron and hydrogen masses, respectively, B := N - Z denotes the neutron excess, and  $\mathcal{E}$  is a suitable parameter set which describes the nuclear

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More generally, we propose that one should define  $E_{LD}$  as the mean trend of the shell-model part of the mass formula; then for any shell correction  $E_{shell} A = 0$ .

shape. Their shell-correction term can describe the shell effects up to fairly large deformations of the nuclear surface. Konecny et al. <sup>6</sup>) have suggested that even the pairing term is shape dependent.

## 2. The shape dependence of the liquid-drop part

The subject of this article is to study the shape dependence of the liquid-drop part of M. Since the Coulomb energy of deformed nuclei was treated by Lawrence  $^{7}$ ) and Flügge  $^{8}$ ), we have to consider only the liquid-drop part resulting from nuclear binding. It consists of (i) the volume term, which is proportional to the volume V or to A and is due to the saturation binding, i.e. constant nuclear density inside the nucleus. (ii) Weizsäcker  $^{1}$ ) introduced the surface term, which is proportional to the surface S or to  $A^{3}$  for spherical nuclei and is a consequence of the assumed analogy to a liquid drop. In 1951, Swiatecki  $^{9,10}$ ) deduced the volume and surface tensions from the Fermi gas model. Later, Knaak, Süssmann, Hilf and Büttner  $^{11}$ ) succeeded in reproducing the experimental value of the surface tension by shell-model calculations with a velocity-dependent potential.

In 1953, Hill and Wheeler <sup>12</sup>) deduced from Fermi gas model that there should exist a curvature-dependent term which is proportional to A<sup>3</sup> as will be seen below, but they obtained an unphysical negative sign for the curvature tension. Recently, Schade and Hilf <sup>13</sup>) have refined this calculation using Swiatecki's "renormalization of the surface position" and arrived at a reasonable positive value. Other approaches to the curvature energy are those of Strutinski and Tyapin <sup>14,15</sup>) and of Myers and Swiatecki <sup>16,17</sup>). Furthermore, their droplet model <sup>16,17</sup>) (a Thomas-Fermi type model) allows as well to calculate the mean values of other physical quantities of the heavy nuclei such as details of the proton- and neutron-distributions, the compressibility and the reduced binding due to the neutron excess.

All the authors established that the curvature energy is linear in the mean total curvature L. This geometrical quantity is an integral over the nuclear surface

$$L := \int dS(R_1^{-1} + R_2^{-1}), \qquad (2)$$

where  $R_1$  and  $R_2$  are the principal radii of curvature of the surface-sheet element dS. This mean total curvature is a quantity of external differential geometry and thus shape dependent. Let us e.g. compare different convex nuclear shapes of equal volume; then L has a minimum for the sphere, just as the quantity surface area has, whereas for arbitrary shapes the shape dependence is different. In contrast to L, there exists another quantity, the well-known Gaussian total curvature  $K := \int dS (R_1 R_2)^{-1}$ , which is a quantity of intrinsic differential geometry; but dK is invariant against bending of the surface sheet. For simple connected closed surfaces, there holds just  $K = 4\pi$  according to a statement of Gauss-Bonnet. Thus K is a constant throughout the fission process and this property, as suggested by Ford  $^{45}$ ) can be successfully used for testing the accuracy of numerical calculations involving  $R_1$  and  $R_2$ .

Within a family of nuclear shapes with equal volume and surface area, the curvature L can still be enlarged as in the case of shapes with long, very thin tubes (e.g. the dumb-bells with rather thin, long necks which has been suggested some time ago as scission-point shapes) or with long thin needles. Therefore, physically, a curvature tension with positive sign would prevent such absurdities by encouraging the nucleus to scission and probibiting porcupine-like shapes.

Geometrically, the quantities volume, surface and curvature are closely connected. They are all three defined as integrals over the surface,  $V := \frac{1}{3} \int dSV \cdot r$ ,  $S := \int dS$  and eq. (2). Furthermore, let us consider a one-parameter family  $\mathcal{S}(s)$  of simple connected, closed, smooth, so-called Steiner sheets, which are parallel; i.e the orthogonal distances of any two sheets  $\mathcal{S}(s_1)$  and  $\mathcal{S}(s_2)$  are universally equal to  $|s_1 - s_2|$  over all the sheets. Not only does V(s+ds) - V(s) = S(s) ds hold, but also as Steiner has proved

$$L(s) = S'(s) = V''(s).$$
 (3)

Thus one can evaluate V and S in terms of a Taylor series, e.g. at  $\mathscr{S}_e := \mathscr{S}(0)$ 

$$V(s) = V_c + sS_c + \frac{1}{2}s^2L_c + \dots, \qquad S(s) = S_c + sL_c + \dots$$
 (4)

Therefore the mean total curvature L should be considered as the natural third-order geometrical quantity describing the total shape of a nucleus.

The hydrostatical energy of the liquid-drop part of the nuclear mass formula is usually described in terms of the geometrical quantities of the "nuclear surface sheet"  $\mathscr{S}_{c}$ . Since the slope of the particle-density distribution n(r) of the actual nuclei is rather smooth, we must carefully elaborate the shape and location of  $\mathscr{S}_{c}$ .

In the case of spherical nuclei, the location of  $\mathcal{S}_c$  is simply defined by its radius. Elton <sup>11</sup>) proposed the nuclear radius to be defined by the expectation value  $\langle r^2 \rangle := (4\pi/Ze) \int dr \, r^4 \rho(r) = \frac{3}{5} R_z^2$ , where  $\rho(r)$  is the charge-density distribution. In an analysis of the electron-scattering experiments of the Stanford group <sup>22</sup>), he established that the maximum particle density, more precisely the proton density, is a constant, which is independent of A, namely  $n_c = 0.168 \, \text{fm}^{-3}$  and obtained  $R_z = r_c A^{\frac{1}{2}} + 2.352 A^{-\frac{1}{2}} + O(A^{-1})$  with  $r_c := (\frac{4}{3}\pi n_c)^{-\frac{1}{2}} = 1.123 \, \text{fm}$ . With this definition, the density of a homogeneous, spherical liquid drop of mass A and radius  $R_z$  is significantly smaller (in third order) than  $n_c$ . However, since  $n_c$  may be regarded as a material constant of nuclear matter, we rather define the nuclear radius as the radius  $R_c$  of a sphere of mass A and density  $n_c$ ,

$$A =: n_{\rm c} V_{\rm c}, \tag{5}$$

thus

$$R_{\rm c}=r_{\rm c}A^{\frac{1}{2}}.$$

This definition can be generalized for arbitrary nuclear shapes and density distributions assuming the conservation of the nuclear volume.

Analogously to n(r), the energy density inside the nuclei is also taken to be a constant  $\eta_c$ , which is independent of A. Furthermore, for the remainder of this section, we assume that in the nuclear surface layer the slopes of the particle density n(r) and of the energy density  $\eta(r)$  do not depend on the local curvature. This resembles the fact given by Elton <sup>18</sup>) that the (90%-10%) thickness of the surface layer of spherical nuclei seems to be independent of A. Then the equidensity sheets are Steiner sheets. The particle- and energy-density distributions can be described by the single parameter s in eq. (3), therefore n(s),  $\eta(s)$ . We choose the parameter s so that  $V(s=0) = V_c$ , thus s=0 denotes the nuclear surface sheet.

Now the hydrostatical energy  $E_{\rm H}$  of the nucleus is

$$E_{\rm H} = \int \mathrm{d}V \, \eta(s) = \int \mathrm{d}s \, S(s) \eta(s). \tag{6}$$

Adding zero to the integrand, namely  $S(s)\{\eta_c\theta(-s)-\eta_c\theta(-s)\}$  and expanding S(s) according to eq. (4), the hydrostatical energy proves to be a sum of a volume, a surface and a curvature term

$$E_{\rm H} = \eta_{\rm c} V_{\rm c} + \sigma S_{\rm c} + \lambda L_{\rm c} + \ldots, \tag{7}$$

where

$$\sigma := \int ds \{ \eta(s) - \eta_c \theta(-s) \}, \qquad \lambda := \int ds \, s \{ \eta(s) - \eta_c \theta(-s) \}. \tag{8}$$

These two moments are just the surface and curvature tension, respectively. Here they only depend on the universal energy-density function  $\eta(s)$  and do not on the shape of the nucleus. Therefore  $E_{\rm H}$  is in fact linear in  $V_c$ ,  $S_c$ , and  $L_c$  as given in eq. (7), if one adopts the assumption that the particle- and energy-density slope is independent of the curvature of the surface. However, this may not be realized in real nuclei; in the more realistic droplet model of Myers <sup>16</sup>), the slopes are dependent on the local curvature dL/dS of the nuclear surface. Thus for the curvature tension, he gets

$$\lambda = \int \mathrm{d}s \left( s + \mathrm{d}S \, \frac{\mathrm{d}}{\mathrm{d}L} \left( \eta(s) - \eta_c \theta(-s) \right) \right).$$

The method used in this work to calculate the hydrostatic energy with the Steiner-sheet assumption is due to Süssmann <sup>19</sup>).

Generally using eq. (5), one can expand eq. (7) in a power series in  $A^{-\frac{1}{2}}$ , namely

$$E_{\rm H} = -\alpha_{\rm c} A + \beta_{\rm c} g(\mathscr{C}) A^{\frac{3}{2}} + \gamma_{\rm c} h(\mathscr{C}) A^{\frac{1}{2}} + \dots$$
 (9)

with the volume, surface, and curvature parameters

$$\alpha_{\rm c} := -\frac{\eta_{\rm c}}{n_{\rm c}} = -\frac{4}{3}\pi r_{\rm c}^3 \eta_{\rm c}, \qquad \beta_{\rm c} := 4\pi r_{\rm c}^2 \rho, \qquad \gamma_{\rm c} := 8\pi r_{\rm c} \lambda, \tag{10}$$

and with the shape-dependent functions

$$g(\mathscr{C}) := S_c/S_0, \qquad h(\mathscr{C}) := L_c/L_0, \tag{11}$$

where  $S_0$  and  $L_0$  denote the surface area and the curvature, respectively, of the sphere of volume  $V_e$ .

Thus, by eqs. (7) and (9), it is shown in a simple model that the dependence of the hydrostatical energy on A and on the deformation of the nucleus is to third order given by the surface area and the mean total curvature of the nuclear density surface, or, more precisely, that there exist two terms of eq. (1), which are just dependent on these geometrical quantities. This agrees with the results obtained by Hill and Wheeler  $^{12}$ ), by Hilf and Süssmann  $^{20}$ ) and by Schade and Hilf  $^{13,21}$ ). It is possible, however, that in eq. (1) there exist other terms which are proportional to  $A^{1}$ , but to first order they will not be curvature dependent but instead are compressibility, diffuseness, and asymmetry terms, which are not included in this simple shell model. These additional terms can be studied in the Thomas-Fermi type droplet model by Myers  $^{16}$ ) and Swiatecki  $^{17}$ ).

# 3. Three methods of fitting the curvature tension

The condensation heat  $-\alpha_e$  and the specific surface tension  $\beta_e$  have often been determined. The approximate values are  $\alpha_e \approx 15$  to 16 MeV and  $\beta_e \approx 17$  to 19 MeV. The main purpose of this paper is to fit the specific curvature tension  $\gamma_e$  to experimental data. There seem to be three possibilities.

- (i) Fit eq. (2) to the experimentally known ground-state masses. Although the first two terms of eq. (2) are much more predominant than the  $A^{\frac{1}{2}}$  term, it is possible by means of a least-squares fit to determine a parameter value for  $\gamma_c h A^{\frac{1}{2}}$ , which will slightly reduce the r.m.s. deviation. But unfortunately the ground-state deformations of most nuclei are very small. Therefore one can determine an  $A^{\frac{1}{2}}$  proportionality but not the shape dependence of  $\gamma_c h$  in this way. It seems to be more sensible to use experimental investigations of the deformations of a given nucleus. Thus A remains constant, whereas the shape of the nucleus changes, therefore the leading first term of eq. (2) does not enter the fit.
- (ii) Schade <sup>21</sup>) determined γ<sub>c</sub> from calculations at the scission point of a fissioning nucleus by fitting the Coulomb-interaction energy to the experimental mean kinetic energies of the fragments by minimizing the potential energy of the nucleus at the scission point and neglecting the kinetic part of the total energy. The kinetic energy at the scission point, however, assumed to be an irrotational non-viscous incompressible flow yields about 20 % of the final kinetic energy of the fragments as has been calculated by Hasse <sup>46</sup>), who after adding the Coulomb-interaction energy obtains the experimental data almost exactly. Futhermore, near the scission point there will be a considerable amount of energy occupied by internal degrees of freedom, which may be in their gross effect described by a finite viscosity. On the other hand, the Coulomb polarization of the fragments cannot be neglected. This is studied by Ryce <sup>47</sup>). Perhaps to some extent, these two effects may cancel each other with regard to the kinetic energies of the fragments. But at least their variances will be enlarged.

(iii) The threshold energy (fission barrier)  $\Delta M$  of a fissionable nucleus is defined as the difference between the saddle-point mass and that of the ground state. As the saddle-point shapes are much more deformed (sausage to dumb-bell like) than the almost spherical ground states, the experimentally known fission barriers should be useful to determine the shape dependence of  $E_{\rm LD}$ . With the Coulomb energy added eq. (7) gives

$$\Delta E_{LD} = \sigma(S_c^S - S_c^G) + \lambda (L_c^S - L_c^G) + (E_{Coul}^S - E_{Coul}^G), \tag{12}$$

where the upper indices S and G refer to the saddle point and the ground state, respectively. The predominant volume term of the mass formula does not enter eq. (12) because  $V_{\rm e}$  and  $\eta_{\rm e}$  are constant throughout the fission process. Unfortunately, however, the shell-correction term of the mass formula does fully enter into  $\Delta M$ , since  $E_{\rm shell}^{\rm S} \approx 0$ , and thus  $\Delta E_{\rm shell} \approx -E_{\rm shell}^{\rm G}$ . Therefore, one must calculate the total  $\Delta M$  and not only its charged liquid-drop part.

We chose the latter method combined with a fit to the ground state masses to determine the specific curvature tension  $\gamma_c$  as described in sects. 6 and 8. The result of our calculations will be that  $\gamma_c$  is in the range 6-8 MeV.

## 4. The mass formula

We adopt the mass formula suggested by Myers and Swiatecki, which is based on their formula of ref. <sup>4</sup>) with the improved shell-correction term of ref. <sup>5</sup>), but we make the following two alterations:

- (i) We add a curvature term as discussed above with a free parameter  $\gamma_e$ .
- (ii) We use the value  $r_c = 1.123$  fm, which Elton <sup>18</sup>) calculated from the charge distributions measured by the Stanford group <sup>22</sup>), whereas Myers and Swiatecki used  $r_c$  as a free parameter which they then fitted to the fission barrier of <sup>201</sup>Tl, and simultaneously fitted the other parameters to the ground-state masses of the beta-stable nuclei. Thus with Elton's value, we seem to get more realistic Coulomb energies.

Because of these alterations, it is necessary to refit all free parameters of the mass formula, especially those of the liquid-drop part. In this work, however, we adopt the values given by Myers and Swiatecki for the parameters of the shell-correction term and the parameter  $\kappa$ . Thus we obtain

$$M(A, B, \mathscr{C}) = M_{n} N + M_{H} Z$$

$$+\left\{-\alpha_{c}A+\beta_{c}g(\mathscr{C})A^{\frac{3}{2}}+\gamma_{c}h(\mathscr{C})A^{\frac{1}{2}}\right\}\cdot\left\{1-\kappa(B/A)^{2}\right\}+E_{\text{Coul}}+E_{\text{shell}}+E_{\text{pair}},\quad(13)$$

with the neutron and hydrogen masses  $M_n = 8.07144$  MeV,  $M_H = 7.28899$  MeV and  $\kappa = 1.7826$ . The special calculations of  $E_{\text{Coul}}$ ,  $E_{\text{shell}}$  and  $E_{\text{pair}}$  are explained in appendix 1. As free parameters, there remain  $\alpha_c$ ,  $\beta_c$ , and  $\gamma_c$ , which will be determined below.

#### 5. Parametrization

Instead of the deformation parameters used by Myers and Swiatecki, we describe the nuclear surface by means of cylinder coordinates  $(\rho, \zeta)$  with  $\rho := F(\zeta)$  and, as suggested by Hasse<sup>23</sup>)

$$F^{2}(\zeta) := \Omega(\zeta_{0}^{2} - \zeta^{2})(\zeta_{2}^{2} + (\zeta - \zeta_{1})^{2}), \tag{14}$$

where  $\Omega$  guarantees the conservation of the unity volume  $\frac{4}{3}\pi$  and  $\Omega = \{\zeta_0^3(\frac{1}{3}\zeta_0^2 + \zeta_1^2 + \zeta_2^2)\}^{-1}$ . Thus  $\zeta$  is a dimensionless coordinate, the dimensioned coordinate is  $z := r_e A^{\frac{1}{3}}\zeta$  and thus  $F(z) = r_e A^{\frac{1}{3}}F(\zeta)$ . The length of the drop is then given by  $2r_e A^{\frac{1}{3}}\zeta_0$ ; the asymmetry is described by  $\zeta_1$ , and  $\zeta_2$  is a measure for the constriction of the drop; for  $\zeta_2 \to \infty$ , one gets spheroidal shapes, whereas for  $\zeta_2 = 0$ , one gets scission at the point  $\zeta = \zeta_1$ . We note the centre of mass at  $\zeta_5 = \frac{2}{3}\Omega\zeta_1\zeta_0^5$ . Following a suggestion by Süssmann <sup>36</sup>), it appears that some of the disadvantages of this otherwise rather useful and simple Hasse parameter set can be removed if one would transform them to  $\mathcal{X} := (\xi_2, \xi_3, \xi_4)$  namely the constriction parameter

$$\xi_2 := \frac{1}{2}\zeta_2^{-2} + \frac{43}{14}(\zeta_0 - 1),$$

the asymmetry parameter

$$\xi_3 := \frac{2}{3}\zeta_1\zeta_2^{-2},$$

and the elongation parameter

$$\xi_4 := \frac{24}{35}(\zeta_0 - 1).$$

This new set  $\mathscr{X}$  has the desired properties (i) to be equal to (0,0,0) for the sphere, (ii) for small deviations from the sphere and under the condition of volume conservation, it is just equal to the usual coefficients  $\mathscr{A} = (\alpha_2, \alpha_3, \alpha_4)$  of the Legendre polynomials of  $P_2$ ,  $P_3$ ,  $P_4$  at least near the central point  $\zeta = 0$ , therefore  $\xi = \alpha$ , if  $(|\xi|, \zeta) \ll 1$ , where now asymmetry and constriction are no longer correlated, (iii) the scission line is in fact the border  $(\xi_2, \xi_3) = \infty$  of the  $\xi_2, \xi_3$  fission process plane.

In this paper, however, we use the Hasse parameters mentioned above and restrict ourselves to reflection-symmetric shapes, i.e.  $\zeta_1 = 0$ . The shape-dependent functions  $g(\mathcal{C})$ ,  $h(\mathcal{C})$ ,  $E_{\text{Coul}}$  and  $E_{\text{shell}}$  are listed in appendix 2.

The ground-state shape of the nucleus is assumed to be a spheroid,  $\zeta_2^{-1} = 0$ . Thus in order to obtain the ground-state mass  $M^G$ , we merely have to minimize  $M(A, B, \mathcal{C})$  with respect to  $\zeta_0$ . The saddle-point deformation, which we take to be symmetrical, was determined according to a method suggested by Lawrence <sup>7</sup>). All numerical calculations were performed on the IBM 7094 computer of the Deutsches Rechenzentrum Darmstadt.

Fig. 1 shows the energy surface of  $^{235}$ U plotted versus  $\zeta_0$  and  $\zeta_2$ . In addition, we have marked the location of the saddle point for different values of the parameters  $\beta_c$  and  $\gamma_c$ , which are thus chosen that the correct fission barrier of 5.75 MeV is always reproduced.

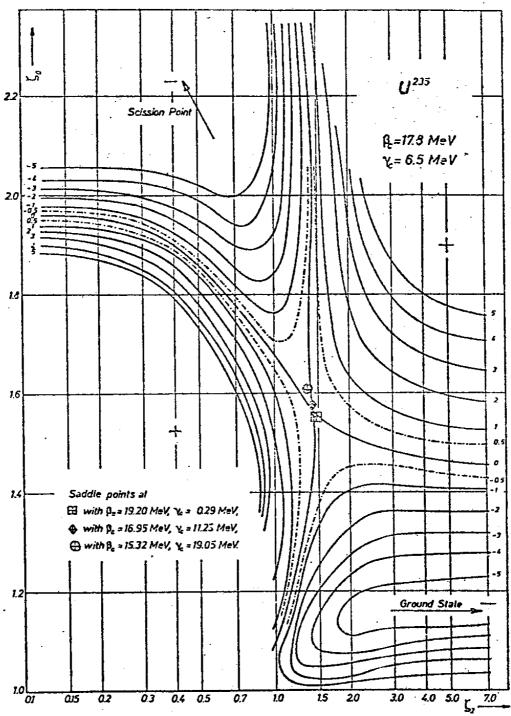
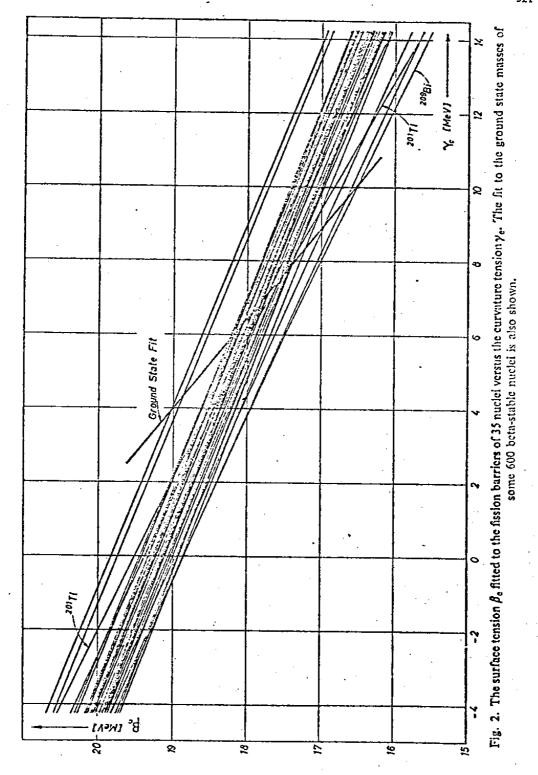


Fig. 1. Energy surface of the nucleus <sup>235</sup>U versus the coordinates of length  $\zeta_0$  and constriction  $\zeta_2$  for symmetric shapes ( $\zeta_1 = 0$ ). The numbers on the contour lines give the deformation energies (in MeV) minus those of the saddle-point configuration and have been calculated with  $\beta_c = 17.8$  MeV and  $\gamma_c = 6.5$  MeV. Different saddle-point configurations are inserted as results of calculations with various values of the parameters  $\beta_c$  and  $\gamma_c$ . Hereby the correct fission barrier of 5.75 MeV is always reproduced.



## 6. Fitting the parameters to the fission barriers

As stated in sect. 2,  $L_c$  has a minimum for constant volume  $V_c$  if the principal radii of curvature  $R_1$  and  $R_2$  are equal, i.e. if the drop is a sphere. If the saddle-point deformation is spheroidal, the curvature term tends to deform the nucleus towards a sphere, i.e. it runs proportional to the surface term. On the other hand, for already constricted shapes, the curvature term favours constriction. The necked-in area almost does not contribute to L because of the opposite signs of the two curvature radii. Therefore, the curvature tension then acts oppositely to the surface tension. Hence the fit of  $\gamma_c$  will be best for nuclei with constricted saddle-point deformations.

The theoretical fission barrier AM is defined as

$$\Delta M^{\text{th}} = \{ \beta_{c}(g^{S} - g^{G})A^{\frac{1}{2}} + \gamma_{c}(h^{S} - h^{G})A^{\frac{1}{2}} \} \left\{ 1 - \kappa \left( \frac{B}{A} \right)^{2} \right\} + (E_{\text{Coul}}^{S} - E_{\text{coul}}^{G}) + (E_{\text{shell}}^{S} - E_{\text{shell}}^{G}).$$
 (15)

For any  $\gamma_c$  in the reasonable range  $-5 \le \gamma_c \le 16$  MeV, one can reproduce the experimental fission barriers  $\Delta M^{exp}$  of a given nucleus, i.e.

$$\Delta M^{\rm th} = \Delta M^{\rm exp},\tag{16}$$

if only  $\beta_c$  is adjusted properly. Solving eqs. (15) and (16) with respect to  $\beta_c$  leads to

$$\beta_{C} = -\gamma_{C} \frac{h^{S} - h^{G}}{g^{S} - g^{G}} A^{-\frac{1}{2}} + \{\Delta M^{exp} - (E^{S}_{Coul} - E^{G}_{Coul}) - (E^{S}_{shell} - E^{G}_{shell})\} \times \left\{ \left[ 1 - \kappa \left( \frac{B}{A} \right)^{2} \right] (g^{S} - g^{G}) A^{\frac{3}{2}} \right\}^{-1}.$$
 (17)

By plotting  $\beta_c$  versus  $\gamma_c$  as fitted to the experimental fission barriers quoted by Myers and Swiatecki<sup>4</sup>), we hope to find a confined area where all the lines intersect.

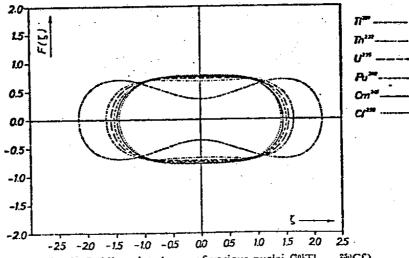


Fig. 3. Saddle-point shapes of various nuclei (201Tl... 250Cf).

This intersection area would then furnish an estimate of the  $(\beta_e, \gamma_e)$  pair, which inserted into eq. (15), would reproduce the experimental fission barriers. Fig. 2 is the plot of the fitted  $\beta_e(\gamma_e)$  versus  $\gamma_e$ . They are almost parallel straight lines except for

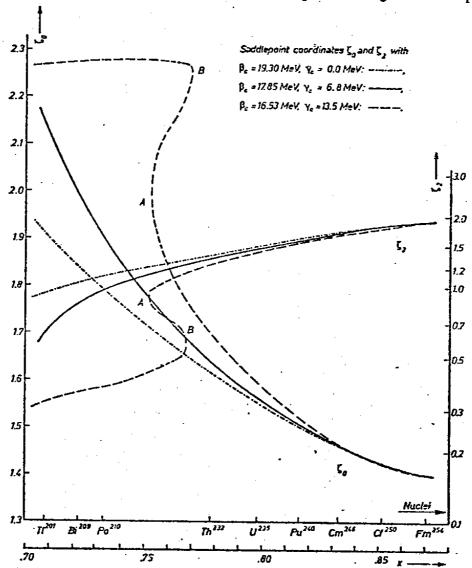


Fig. 4. Saddle-point coordinates  $\zeta_0$  and  $\zeta_1$  for various values of  $\gamma_0$  and  $\beta_0$ . For abscissa, the fissility parameter x has been calculated with  $\beta_0 = 17.85$  MeV and  $\gamma_0 = 6.8$  MeV. The sections (A-B) of the coordinate lines determined with  $\beta_0 = 16.53$  MeV and  $\gamma_0 = 13.5$  MeV describe the coordinates of the minimum between the two saddle points. This topological fact has been brought to our attention by Swiatecki <sup>43</sup>).

<sup>201</sup>Tl and <sup>209</sup>Bi. They run in a rather narrow strip. With an uncertainty of the experimental values ranging from 1.5 MeV (<sup>201</sup>Tl) to say 0.3 MeV for the heavier nuclei,  $\beta_c$  is uncertain to  $\Delta\beta_c \approx 0.3$  MeV, which would result in an overlap of nearly all lines. We also plotted the ground-state fit, which is explained in sect. 8.

#### 7. Discussion

Unfortunately, the saddle-point deformations of most of the nuclei under consideration ( $A \ge 210$ ) are rather sausage like (see fig. 3), thus the curvature term does not yet become effective in the sense that the saddle-point deformations do not change very much with increasing  $\gamma_c$  (see figs. 1 and 4). Therefore, the ratio  $q := (h^S - h^G)/(g^S - g^G)$  of eq. (17) remains nearly constant with increasing  $\gamma_c$  (see fig. 5), thus giving a straight line for each nucleus:

$$\beta_{c} = m_{N,Z} \gamma_{c} + b_{N,Z},$$

$$m_{N,Z} = (h^{S} - h^{G})/(g^{S} - g^{G})A^{-\frac{1}{2}} = qA^{-\frac{1}{2}},$$

$$b_{N,Z} = \{AM^{exp} - (E^{S}_{Coul} - E^{G}_{Coul}) - (E^{S}_{shell} - E^{G}_{shell})\}$$

$$\times \left\{ \left(1 - \kappa \left(\frac{B}{A}\right)^{2}\right) (g^{S} - g^{G})A^{\frac{1}{2}} \right\}^{-1}.$$
(18)

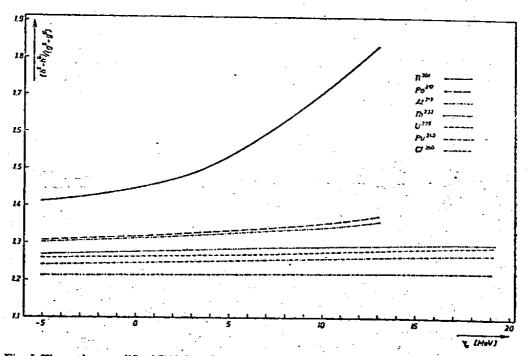


Fig. 5. The ratio  $q := (h^S - h^G)/(g^S - g^G)$  versus the curvature tension  $\gamma_c$ . The surface tension has been chosen in a way to reproduce the fission barriers of the various nuclei correctly.

Furthermore, for deformations in the saddle-point region of all nuclei with  $A \ge 230$ ,  $h(\mathcal{C})$  is still proportional to  $g(\mathcal{C})$ . Thus q ranges only from 1.2 to 1.28 for all nuclei regardless of their saddle-point deformations (see fig. 5). Dividing q by  $A^{\frac{1}{2}}$ , we obtain the gradient  $m_{N,Z}$  which thus ranges from 0.19 to 0.208, i.e. the straight lines in fig. 2 are almost parallel.

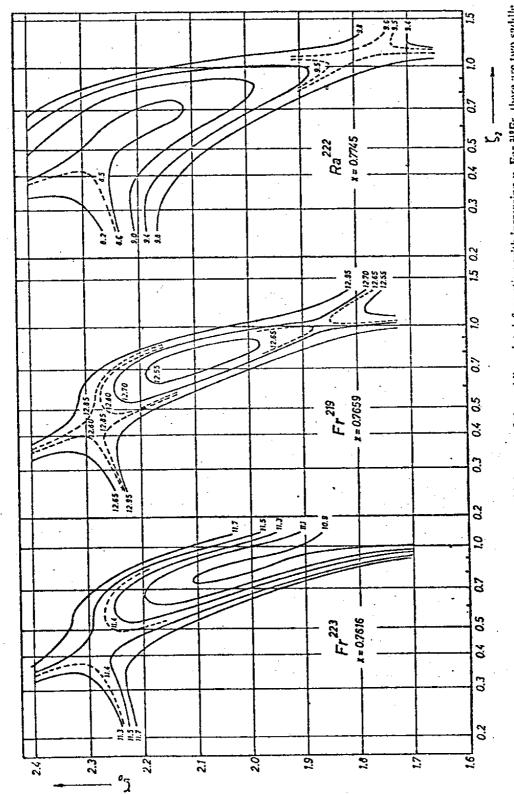
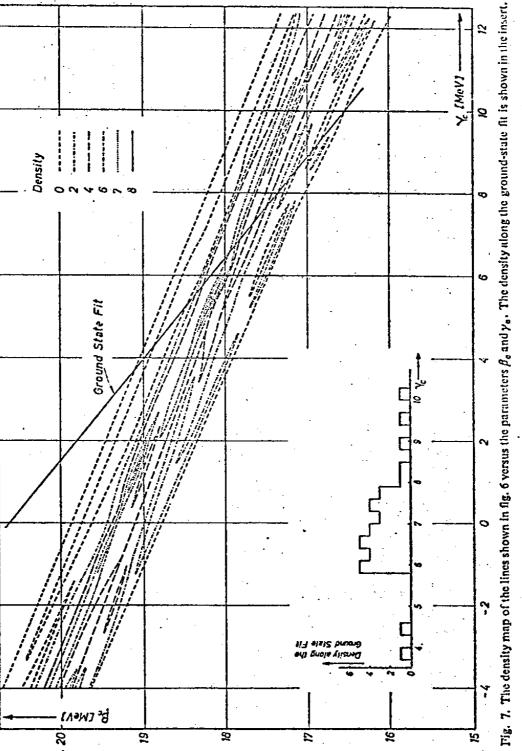


Fig. 6. Energy maps versus  $\zeta_0$  and  $\zeta_2$  showing the rapid decrease of the saddle-point deformation with increasing x. For <sup>318</sup>Fr, there are two saddle points. The numbers on the contour lines give the deformation energies (in MeV) minus those of the ground-state configuration calculated with  $\beta_0 = 16.53$  MeV and  $\gamma_0 = 13.5$  MeV.



Only the saddle-point shapes of the lighter nuclei (A < 220) are constricted and therefore change considerably with  $\gamma_e$ . There can even occur a jump in the saddle-point elongation  $\zeta_0^S$  and constriction  $\zeta_2^S$ , which can be observed in the following ways. If  $\gamma_e$  is constant and sufficiently large ( $\gamma_e \ge 10$  MeV),  $\zeta_0^S$  decreases and  $\zeta_2^S$  increases rapidly with increasing fissility parameter  $^{\dagger}$  x, as shown in figs. 4 and 6, some nuclei having even a double-hump fission barrier showing two saddle points. The same happens when x is kept constant and  $\gamma_e$  increases.

The possible occurrence of double-hump fission barriers in a small fissility parameter area about Ra is strongly correlated to the well-known change in deformation from constricted saddle-point shapes for light nuclei to sausage-like ones for heavy nuclei at that x-area. It proves that this change is emphasized by the curvature tension, and simultaneously the saddle-point area seems to become very flat. Then for sufficiently large values of  $\gamma_e$  even a small second minimum occurs. This is a consequence of the different ways in which surface and curvature tensions act on constricted nuclei. Thus the formation of a Strutinski-minimum  $^{26-30}$ ) in this x-area is fostered in the same degree as the value of the curvature tension is increased. It will depend on detailed extra-polations of the Strutinski shell term  $^{26}$ ) to the strongly constricted and deformed saddle-point shapes in question and on the actual value of  $\gamma_e$  if there will be any nucleus near Ra showing shape isomers.

For the lighter nuclei (e.g.  $^{201}$ Tl and  $^{209}$ Bi), the ratio q changes considerably (see fig. 5), the lines in fig. 2 are slightly bent. Furthermore, the line of  $^{201}$ Tl intersects nearly all other lines within the small range 2-8.5 MeV. Bismuth does not seem to be a good example, because its fission barrier was measured  $^{31}$ ) with a mixture of two isotopes  $^{209}$ Bi and  $^{207}$ Bi, thus its value for  $b_{N,Z}$  of eq. (18) is not very reliable.

TABLE 1

The three areas of maximal intersection density

	γ <sub>c</sub> area (MeV)	β' <sub>c</sub> area (MeV)	Peak value (arbitrary unit)
-	-2.00.5	19.4 19.7	7
	+0.5+2.0	18.9 19.2	8
	+4.4+6.0	18.05 18.35	8

The  $b_{N,Z}$  of eq. (18) ranges from 18.8 to 19.5 MeV and does not show significant dependence on N, Z or A. This scattering is due to the uncertainty of the experimental values  $\Delta M^{\rm exp}$  and also of the shell-correction term. This term is fitted to the ground-state masses, but its shape dependence is somewhat hypothetical for the major deformations at the saddle point. Furthermore, we did not yet refit its parameters. It would be a major improvement however, to have at our disposal a shell-correction term,

$$x := \frac{1}{2}(E_{\text{Coul}}/(E_{\text{surf}} + E_{\text{curv}}))_{\text{sphere}}$$

<sup>†</sup> As the Bohr-Wheeler <sup>24</sup>) fissility parameter does not take the curvature energy into account, we have to modify it as follows [see also Hasse <sup>25</sup>)]

which holds even for large deformations, constrictions and asymmetries of the nuclear shape. This has been performed by a thorough study of Nix <sup>32,33</sup>) using a Nilsson-Strutinski type model.

The very small variations of  $m_{N,Z}$  as well as scattering of the  $b_{N,Z}$  prevent the lines in fig. 2 from intersecting within a small area. For this reason, we first tried to apply statistical methods and counted the number of lines passing through small sections of equidistant lines at right angles to a mean straight line. The density map is plotted versus  $\gamma_e$  and  $\beta_e$  in fig. 7. There are three maxima listed in table 1. These areas yield the most probable values for the pair  $(\beta_e, \gamma_e)$ . The third set seems to be the best, for it includes the fit to  $^{201}$ Tl and the ground-state fit discussed below.

# 8. Fitting the parameters to the ground-state masses

The method of fitting  $\beta_c$  and  $\gamma_c$  to the experimental fission barriers has produced only a somewhat vague determination for these parameters. The lines in fig. 2 do not have a definite single intersection point or intersection density maximum because of the lack of experimental threshold energies of lighter nuclei. We therefore here combine this fit with the natural postulation that our mass formula should also reproduce the experimental ground-state masses  $M^{exp}$  with the same  $\beta_c$  and  $\gamma_c$  values.

We roughly evaluated the constants  $\alpha_e$  and  $\beta_e$  for given  $\gamma_e$  by means of the least-squares fit to the 600 ground-state masses quoted in ref. <sup>4</sup>). Here we always chose  $\beta_e$  and  $\gamma_e$  so that it was on the maximum intersection-density line of the fission barrier fit. Starting with estimated values for  $\alpha_e$  and  $\beta_e$ , we sought the minimum of  $M(A, B, \mathcal{C})$  for each nucleus with regard to deformation (varying  $\zeta_0$  with  $\zeta_2 = \infty$ ), i.e. the theoretical ground-state mass  $M^{th}$ ; leaving the specific shape of each nucleus fixed for the minimum of  $\sum_{Z,N} (M^{th} - M^{exp})^2$  with respect to  $\alpha_e$  and  $\beta_e$ . With these values, we began a new iteration until the process converged. Thus we found the following dependence of the parameters  $\beta_e$  and  $\alpha_e$  on  $\gamma_e$ :

$$\beta_c(\gamma_c) = 20.632 \text{ MeV } -0.4093\gamma_c,$$

$$\alpha_c(\gamma_c) = 16.277 \text{ MeV } -0.0409\gamma_c.$$
(19)

Figs. 2 and 7 show the line  $\beta_c(\gamma_c)$  denoted as the ground state fit. Both the ground state and fission-barrier fits of the heavy nuclei and <sup>201</sup>Tl yield a curvature tension of approximately 6 to 8 MeV, the most probable value being  $\gamma_c = 6.8$  MeV, then  $\beta_c = 17.849$  MeV and  $\alpha_c = 15.999$  MeV.

Starting with eqs. (9) and (19), one gets for superheavy nuclei, being almost spherical,

$$E = E_0 + \Delta E, \tag{20}$$

where  $E_0$  is the nuclear mass without taking a curvature tension into account and  $\Delta E$  is the lack of binding due to a curvature tension  $\gamma_c$ ,

$$\Delta E := \gamma_c F(A), \qquad F(A) := (0.0409A - 0.4093A^{\frac{1}{2}} + A^{\frac{1}{2}}).$$
 (21)

Due to eq. (19), volume and surface tensions are adjusted to every value of  $\gamma_c$  to fit best the known ground-state masses. For all superheavy nuclei, the lack-function F(A) is positive,

$$F_{\rm sh}(A) \approx \frac{1}{142}A - \frac{104}{71}$$
 (22)

in that area, i.e. the binding of all superheavy nuclei is reduced when taking curvature tension into account. As an example, for A = 278 we get F(A) = 0.49 and with  $\gamma_c = 6.8$  MeV, finally  $\Delta E = 3.34$  MeV.

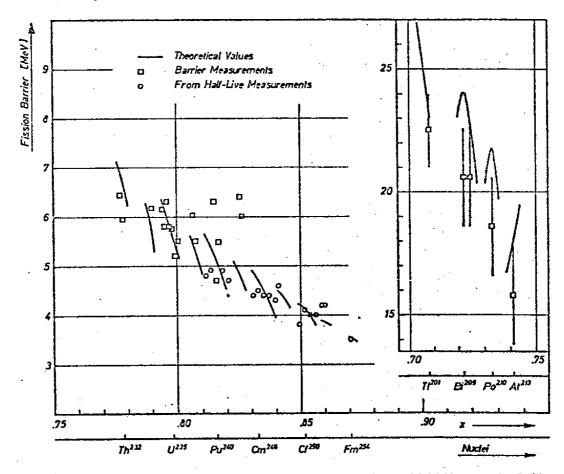


Fig. 8. The fission barriers calculated with  $\beta_c = 17.849$  MeV and  $\gamma_c = 6.8$  MeV versus the fissility parameter x. For comparison, the experimental values 4) are shown.

With the values of  $\alpha_c$ ,  $\beta_c$ , and  $\gamma_c$  mentioned above, we calculated the fission barriers; the results shown in fig. 8 demonstrate a very good agreement between the theoretical and experimental values. In the region of the magic numbers Z=82 and N=126, i.e. Bi and Po, the effect of the shell-correction term seems to be too large. For more detailed investigations, however, further experimentally determined fission barriers are needed. Also, in the region of Pu and Cm, the theoretical line in fig. 8

seems to be too steep. We interpret these two effects as being due to the shell-correction term, since near the magic numbers the bulges of the Myers-Swiatecki term of ref.<sup>5</sup>) seem to be still too steep.

The agreement between the theoretical and the experimental ground state masses, however, is not striking, the r.m.s. deviation being 2.8 MeV. A fit of  $\alpha_c$ ,  $\beta_c$  and  $\gamma_c$  only to the experimental ground-state masses gives  $\alpha_c = 16.723$  MeV,  $\beta_c = 25.09$  MeV and  $\gamma_c = -10.9$  MeV with a r.m.s. deviation of 1.45 MeV. If the parameter  $\kappa$  is fitted as well, then  $\alpha_c = 16.789$  MeV,  $\beta_c = 25.34$  MeV,  $\gamma_c = -10.7$  MeV and  $\kappa = 1.833$  with a 1.3 MeV r.m.s. deviation. Even with these values, there remain deviations from the experimental ground state masses which show significant shell effects. This indicates the necessity of refitting the shell-correction parameters as well.

Furthermore, the  $r_c$  determination of Elton should be recalculated and would probably lead to a somewhat larger value. Seeger <sup>34</sup>) thoroughly fitted all experimentally available data on nuclear masses and obtained a  $r_c$  value of about 1.175 fm. This agrees fairly well with the mean nuclear elementary radius  $r_0$  calculated by Myers <sup>35</sup>) from his droplet model. He proved as well that the proton-radius  $r_p$  should be about 4% smaller than  $r_0$ ; therefore  $r_p$  is in the range of the  $r_c$  of Elton, but in the liquid drop terms mentioned in this paper one should use the elementary radius  $r_0$  of Myers. We hope that this will reduce very much the r.m.s. deviation mentioned above.

Our result of 6-8 MeV for  $\gamma_c$  agrees fairly accurately with other calculations, e.g. Schade and Hilf <sup>13</sup>) obtained from simple Fermi gas model calculations the range 1.9  $\lesssim \gamma_c \lesssim 13$  MeV. In a preliminary calculation using the above mentioned geometrical assumption on the nuclear density surfaces, Süssmann <sup>36</sup>) obtained  $\gamma_c \approx 3$  MeV from the shell model. From scission-point calculations by fitting the Coulombinteraction energy to the experimental mean kinetic energies of the fragments Schade <sup>21</sup>) obtained 16 MeV, which seems a little high, but he did not refit the surface parameter  $\beta_c$  and uses  $r_c = 1.2249$  fm as quoted by Myers and Swiatecki <sup>5</sup>). Myers and Swiatecki <sup>17</sup>) started with a two-nucleon potential and obtained  $\gamma_c \approx 9.34$  MeV from their droplet model.

### 9. Conclusion

Although there may be several terms proportional to  $A^{\frac{1}{2}}$  in the mass formula, e.g. curvature energy, compressibility and part of the shell term, they can be distinguished by studying adjusted physical processes. For the curvature term, they are the fission barriers. For this reason, threshold energies of lighter nuclei such as Bi with more constricted saddle-point shapes should be measured. This has been performed  $^{37}$ ) in the meantime.

We have used the fixed value  $r_c = 1.123$  fm instead of fitting it as a free parameter, which would lead to somewhat larger values of about 1.15-1.2 fm. This of course has strengthened the Coulomb energy which forces the nucleus to become more deformed. With regard to deformations, this effect is mainly compensated by a positive curvature tension, whereas the surface tension remains about the same, as we obtained by

fitting these parameters to the experimental fission barriers. With regard to the overall trend of the ground-state masses, however, the larger Coulomb energies are compensated in the binding energy first by a larger value of  $\alpha_c$ , which is obvious and secondly by a negative value of  $\gamma_e$  and a larger value of  $\beta_e$ . The latter we believe to be due to the shell-correction term of Myers and Swiatecki and the method by which they determined its parameters; they fitted them to the difference between the experimentally known ground-state masses and the calculated liquid-drop masses. Thus the expression  $-cA^{\frac{1}{2}}$  of the shell-correction term (see appendix I) fixes this term to the overall trend of the theoretical liquid-drop part. As we altered  $r_c$ , this trend changed, therefore c should have been refitted. By preliminarily using the original c-value, the A<sup>1</sup> dependence of the shell-correction term was partly transferred to that of the liquiddrop term, therefore the "curvature tension" of  $\gamma_c = -11$  MeV obtained by our ground-state fit does not only result from curvature effects but includes shell effectsas well. We hope that by a new thorough fitting both, the liquid-drop and the shellcorrection-term parameters, the discrepancy between the values determined by the fitting to the fission barriers and those of the ground-state fit will be diminished.

Furthermore, the functional dependence of the shell-correction term on N and Z and the deformation of the nuclei should be the subject of further investigations. Hilf and Süssmann <sup>19</sup>) obtained from Fermi gas model calculations that the shell-correction part may not contain an  $A^{\dagger}$  term. Süssmann et al. <sup>38</sup>) recently proposed another formula where the shell energy is based on the magic numbers and the local curvature of the nuclear surface. With this term, shell effects of even extremely deformed nuclei can be defined.

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### Appendix 1

CALCULATIONS OF Ecout, Eshell AND Epatr

According to Myers and Swiatecki <sup>4,5</sup>), we calculated the Coulomb energy  $E_{\text{Coul}}$ , the shell-correction term  $E_{\text{shell}}$ , and the pairing energy  $E_{\text{pair}}$  as follows:

$$E_{\text{Coul}} = \frac{3}{5} \frac{Z^2 e^2}{r_c A^{\frac{1}{5}}} f(\mathcal{C}) - \frac{1}{2} \pi^2 \left(\frac{d}{r_c}\right)^2 \frac{Z^2 e^2}{r_c A}, \qquad (23)$$

† Then at the Institut für Theoretische Physik, Universität Frankfurt/M., Germany.

with  $r_c = 1.123$  fm (in contrast to the  $r_c = 1.2249$  fm of Myers and Swiatecki) and d = 0.5461 fm the surface thickness parameter in a Fermi-type density distribution, and

$$f(\mathcal{C}) = \frac{5}{3} \frac{R_c}{V_c^2} \frac{1}{2} \int dr_1 \int dr_2 \theta(R_c - r_1) \theta(R_c - r_2) / |r_1 - r_2|.$$
 (24)

The shell-correction term is

$$E_{\text{shell}} = C\{(G(N) + G(Z))(\frac{1}{2}A)^{-\frac{1}{2}} - cA^{\frac{1}{2}}\}(1 - 2\theta^2) \exp(-\theta^2), \tag{25}$$

with C = 5.8 MeV, c = 0.325 and

$$G(X) := \frac{3}{5} \{ (M_i^{\frac{5}{2}} - M_{i-1}^{\frac{3}{2}})(X - M_{i-1}) / (M_i - M_{i-1}) - (X^{\frac{5}{2}} - M_{i-1}^{\frac{3}{2}}) \}, \tag{26}$$

for  $M_{i-1} \leq X \leq M_i$ , and the magic numbers  $M_i = 2$ , 8, 14, 28, 50, 82, 124, 184. The factor  $\theta^2$  is the Myers-Swiatecki measure for the deformation of the nucleus. With its surface described by the radius  $R(9, \varphi)$  and the radius of the sphere of equal volume by  $R_c$ , then

$$\theta^2 := (4\pi a^2)^{-1} \int d\Omega (R(\theta, \varphi) - R_s)^2, \qquad \frac{a}{r_s} = 0.444.$$
 (27)

The pairing energy is defined as usual for spherical nuclei:

$$E_{\text{pair}} := \begin{cases} 11A^{-\frac{1}{2}} \text{ MeV for doubly odd nuclei} \\ 0 \text{ MeV for odd-mass nuclei} \\ -11A^{-\frac{1}{2}} \text{ MeV for even nuclei.} \end{cases}$$
 (28)

In this paper we have used this simple pairing term. But one should be aware, that the pairing term is somewhat shape dependent. At least for nuclei lighter than Ra, the pairing energy of the saddle point should be about the sum of the pairing terms of the two fragments. A first-order correction to this equation can be calculated from the molecular fission model of Kennedy <sup>39</sup>) and Nörenberg <sup>40</sup>). Experimentally, the shape dependence of the pairing energy has been determined by Konecny et al. <sup>41</sup>), Moretto, Thompson, Khodai-Joopari et al. <sup>37,42</sup>). These replacements of eq. (28) will certainly improve the mass formula.

#### Appendix 2

## THE SHAPE-DEPENDENT FUNCTIONS

With the parameter set  $\mathscr{C} = (\zeta_0, \zeta_1, \zeta_2)$  which describes the nuclear surface, the shape-dependent functions of sect. 5 are as follows (the prime denoting differentiation with respect to  $\zeta$ ):

The surface function  $g(\mathscr{C})$  is

$$g(\mathscr{C}) := \frac{S_c}{S_0} = \frac{1}{2} \int_{-\zeta_0}^{\zeta_0} d\zeta F(\zeta) (1 + F'^2(\zeta))^{\frac{1}{2}}. \tag{29}$$

With  $L := \int dS(R_1^{-1} + R_2^{-1})$  and  $R_1 = -(1+F'^2)^2/F''$  and  $R_2 = F(1+F'^2)^2$ , the curvature function  $h(\mathcal{C})$  is obtained

$$h(\mathscr{C}) := \frac{L_{\rm e}}{L_{\rm o}} = \frac{1}{4} \int_{-\zeta_{\rm o}}^{\zeta_{\rm o}} d\zeta (1 + F'^{2}(\zeta) - F(\zeta)F''(\zeta))(1 + F'^{2}(\zeta))^{-1}, \tag{30}$$

or integrating by parts 14)

$$h(\mathscr{C}) = \frac{1}{4} \int_{-\zeta_0}^{\zeta_0} d\zeta \, F' \arctan F', \tag{31}$$

without the need of calculating F''.

The Coulomb-energy function according to Lawrence 7) is

$$C(\mathscr{C}) = \frac{15}{4}\pi \int_{0}^{2\zeta_{0}} d\zeta \int_{0}^{1} dy \int_{0}^{\pi} d\varphi \frac{\zeta F_{1}^{2} F_{2}^{2} \sin^{2} \varphi}{\zeta(1-y) + (\zeta^{2}(1-y)^{2} + F_{1}^{2} + F_{2}^{2} - 2F_{1} F_{2} \cos \varphi)^{\frac{1}{2}}}, \quad (32)$$

with  $\zeta := \zeta + \zeta_0$  and  $F_1(\zeta) := F(\zeta - \zeta_0)$  and  $F_2(\zeta) := F(\zeta y - \zeta_0)$ . Finally, since  $R_c = r_c A^{\frac{1}{2}}$  and  $R = R_c (F^2(\zeta) + \zeta^2)^{\frac{1}{2}}$  and  $\cos \vartheta = \zeta (F^2(\zeta) + \zeta^2)^{-\frac{1}{2}}$ , one gets

$$\theta^{2} = \frac{1}{2} \frac{R_{c}^{2}}{a^{2}} \int_{-\zeta_{0}}^{+\zeta_{0}} d\zeta \frac{F(\zeta)(F(\zeta) - \zeta F'(\zeta))\{(F(\zeta) + \zeta^{2})^{\frac{1}{2}} - 1\}^{2}}{(F^{2}(\zeta) + \zeta^{2})^{\frac{3}{2}}}.$$
 (33)

Ail integrations were performed numerically by means of a 24-point Gauss-Legendre technique <sup>13</sup>) with one division of the integration interval.

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