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FISSION BARRIERS WITHIN THE LIQUID DROP MODEL WITH THE SURFACE-CURVATURE TERM

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The recently revised liquid drop model (PRC 67(2003) 044316) containing the curvature term reproduces the masses of 2766 experimentally known isotopes having $Z \geq 8$ and $N \geq 8$ with the r.m.s. deviation equal to 0.698 MeV when the microscopic corrections of Moeller *et al.* is used. The influence of the congruence energy as well as the compression term on the barrier heights is discussed within this new macroscopic model. The r.m.s. deviation of the fission barrier heights of 40 isotopes with $Z \geq 34$ is 1.73 MeV only when deformation-dependent congruence energy is included. The effect of the compression term in the liquid drop energy has rather weak influence on the barrier heights.

1. Introduction: General Framework

The newly developed Lublin-Strasbourg-Drop (LSD) model[1] for the macroscopic part of the binding energy of nuclei reproduces the experimentally known masses of 2766 isotopes[2] with $Z \geq 8$ $N \geq 8$ with an accuracy better than other macroscopic-microscopic[3] or selfconsistent models known up to date. The mean-square deviation of the experimental *vs.* theoretical (LSD) masses is 0.698 MeV only when one includes the shell, deformation and pairing corrections of Ref. 4 and the congruence energy from Ref. 3. For illustration, the deviations of the masses calculated within the LSD approach from the experimental ones are presented in Fig. 1, where the points corresponding to the different isotope chains are connected by solid lines. The LSD mass expression differs from the traditional Myers and Świątecki liquid drop mass formula[5] in that it contains the first order curvature term (proportional to $A^{1/3}$) as well as in terms of the parameter values that are fitted to the present-day experimental data. The LSD mass formula for the macroscopic part of the binding

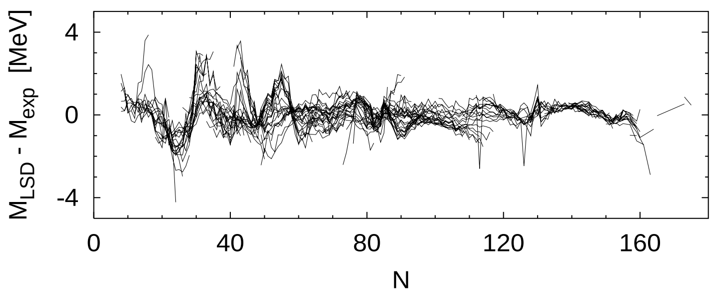

Fig. 1. Deviation of theoretical masses and the experimental as function of the neutron number. The points corresponding to the different isotopes chains are connected.

energy, expressed in MeV, has the following form

$$\begin{aligned} E_{\mathrm{LSD}}(A, I; \mathrm{def}) = & -15.4920\,(1-1.8601\,I^{\,2})\,A \\ & +16.9707\,(1-2.2938\,I^{\,2})\,A^{2/3}\,B_{\mathrm{surf}}(\mathrm{def}) \\ & +3.86020\,(1+2.3764\,I^{\,2})\,A^{1/3}\,B_{\mathrm{cur}}(\mathrm{def}) \\ & +3/5e^2Z^2/(1.21725\,A^{1/3})\,B_{\mathrm{Coul}}(\mathrm{def}) - 0.9181\,Z^{\,2}/A + E_{\mathrm{cong}}\,, \end{aligned} \tag{1}$$

where $I = (N-Z)/A$ and $A = N+Z$. The deformation dependent functions B_{surf}, B_{cur} and B_{Coul} are defined as ratios of the surface, average curvature and Coulomb energies, respectively, and the corresponding quantities evaluated for a sphere of the same volume and charge. The congruence energy term (in MeV) according to Ref. 3 is equal to:

$$E_{\mathrm{cong}} = -10 \cdot \exp(-4.2\,|I|)\,. \tag{2}$$

2. Fission Barriers within LSD

It turns out that the liquid drop model which in addition to the volume, surface and Coulomb energies contains just the first order curvature term gives not only a very good description of the masses but also a rather satisfactory prediction of the fission barrier heights[a] as it is seen from Fig. 2, where the Thomas-Fermi[3] and LSD barrier heights are compared with the experimental data, cf. Refs. 3, 6, 7. It is worth emphasizing that all the parameters of the LSD model were fitted to the nuclear masses only and thus the correct reproduction of the barrier heights can be seen as an additional sign of the intrinsic consistency of the model.

The mean square deviation of the barrier heights from experiment is $\langle \delta V_B \rangle = 3.56$ MeV, but it decreases to only 0.88 MeV when the four lightest nuclei are disregarded i.e. when only the nuclei with $Z > 70$ are considered. It is

[a]In this article we use the same definition of the barrier height as the one in Ref. 3; we define the barrier height as the difference between the macroscopic mass of a nucleus evaluated in the saddle point and its theoretical mass in the ground state, i.e. we assume that the shell and pairing corrections at the saddle points are negligibly small.

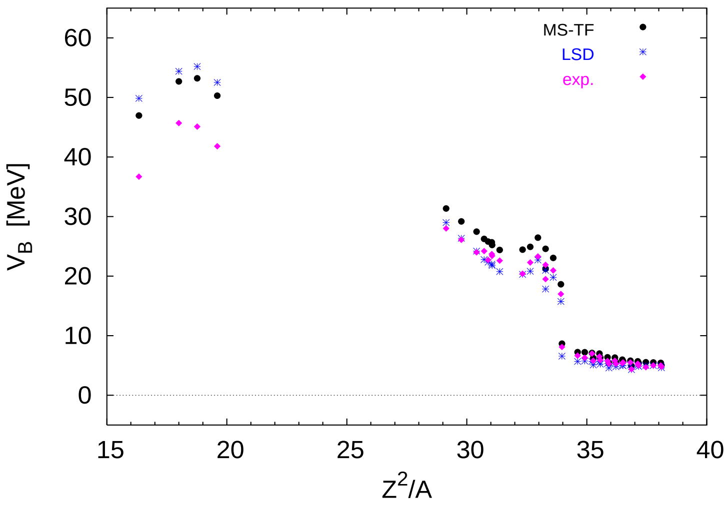

Fig. 2. Experimental fission barrier heights compared to the theoretical ones obtained with the LSD and the Thomas-Fermi models as a function of the fissility parameter.

seen from Fig. 2 that for heavier nuclei the agreement between the experimental data and the LSD fission barriers is even better than that for the MS-TF model, while for the light isotopes ($A < 100$) both models give comparable fission barriers, approximately 10 MeV too high. This large discrepancy between the theoretically predicted fission barrier heights and the measured values for light nuclei could originate from the fact that the fission barriers of these light nuclei are very broad and the saddle points are very close to the scission points. At such configurations it happens that the negative congruence energy (nearly) doubles, as suggested in Ref. 8, and as a consequence the fission barrier heights calculated using such an approach could be much closer to the experimental ones. The deformation dependence of the congruence energy (2) developed in Ref. 8 for the fission of a Hill-Wheeler box is

$$E_{\rm cong}(I, {\rm def}) = -(2 - R_n/\bar{R}_f) \cdot 10 \exp(-4.2I)\,{\rm MeV}\,, \tag{3}$$

where R_n is the neck radius and $\bar{R}_f$ is the average radius of the fission fragments to be born.

The effect of the deformation dependence of the congruence energy on the barrier heights is seen in Fig. 3, where the difference between the original (i.e. without the congruence contribution) and the modified one (i.e. with the congruence contribution) theoretical LSD and the experimental barrier heights are plotted. The LSD estimates of the barrier heights are much closer to the experimental data for light nuclei when the deformation dependence of the congruence energy is taken into account. The results for the heaviest nuclei remain nearly unchanged because the saddle point for such nuclei is very far from the scission configuration.

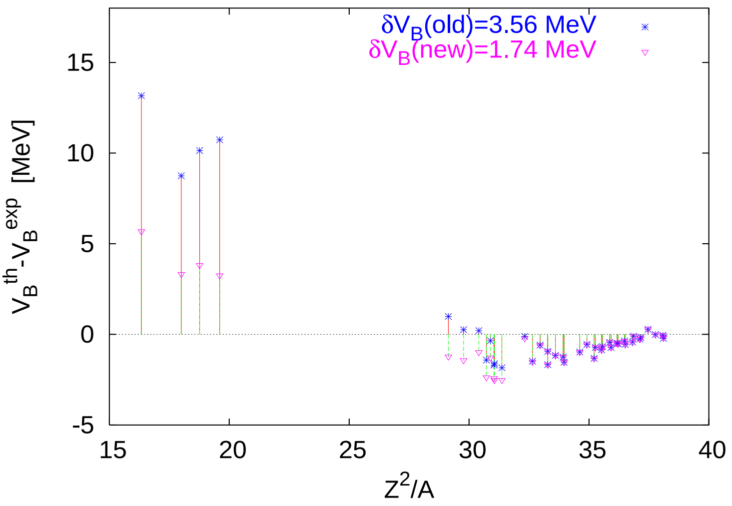

Fig. 3. Differences between the theoretical (LSD) and the experimental fission barrier heights as a function of the fissility parameter, "old" - without, "new" - with the congruence contribution.

3. Estimates of the Compression Energy Contributions

A few remarks will be in place here, related to the magnitude of the compression energy contribution that, like the contribution from the curvature term, is proportional to $A^{1/3}$. Our parameterization that uses the term proportional to $b_{\rm cur}$ (see below) corresponds more to the discussions usually associated with the liquid drop energy expression rather than the one used in the droplet model approach. Here we will deviate from the main line of the paper and introduce the energy expression that is not difficult to obtain on the basis of the droplet model; it gives in an approximate way the deformation dependent compression term. The correspondence between the two types of parameterizations has the form[9]

$$b_{\rm cur}\,(1-\kappa_{\rm cur}\,I^{\,2})B_{cur}(def)\,A^{1/3} \tag{4}$$

$$\Downarrow$$

$$\begin{aligned}&\tilde{b}_{\rm cur}(1-\tilde{\kappa}_{\rm cur}I^{\,2})B_{cur}(def)A^{1/3} \\ &-\frac{2}{K}\cdot\left[\tilde{b}_{\rm surf}(1-\tilde{\kappa}_{\rm surf}I^{\,2})B_{surf}(def)\right]^2\cdot\left[1-x\,\frac{B_{Coul}(def)}{B_{surf}(def)}\right]^2 A^{1/3}\,,\end{aligned} \tag{5}$$

where K denotes the nuclear matter incompressibility coefficient and x fissility parameter. While increasing the curvature increases the energy contribution to the binding, the corresponding modification of the compressibility is of the opposite sign reflecting the fact that the number of neighbors of a given particle in the related surface region decreases.

To estimate the typical order of magnitude in the energy contributions we could use transformation (5) that implies $b_{\rm cur} \approx 7$ MeV; this estimate can be compared to the results that can be found in the literature: Ref. 10 quotes the estimate $b_{\rm cur} \approx 11$ MeV, while Ref. 11 uses $b_{\rm cur}$ ranging from 9.52 to about 13 MeV as obtained with the six representative Skyrme interactions; one may conclude that our fit result and the quoted microscopic model results have comparable orders magnitude, our numbers being slightly smaller.

Making the estimates illustrated in Table 1 below we have used the value of $K = 234$ MeV for the compressibility parameter estimated in Ref. 3 within the Thomas-Fermi model and the curvature and surface coefficients as in Table 1.

As it is seen from the results in Table 1 where examples of a few nuclei illustrative for various mass ranges are given, the differences between the binding energies predicted including or not including the compression energy contribution are indeed rather small: in the considered examples they vary between 2 and 64 keV. By subtracting the shell correction energies in order to reduce the problem to a discussion of energy contributions at spherical shapes (as we and other authors do) one introduces the uncertainties related to the shell corrections themselves, the latter being at best comparable to- if not markedly larger than the corresponding numbers in the Table. It then follows that the effect of neglecting this contribution when fitting the parameters to the nuclear binding energies is very small indeed and it was not taken into account in the mass fitting procedures.

The effect on the fission barrier heights amounts to only 0.02 MeV for ^{252}Cf and neighboring nuclei and to $\sim$1.5 MeV (i.e. $\sim$3%) for the isotopes with $A \approx 100$ - these contributions are smaller than the expected uncertainties related to the congruence contributions and were not taken into account when constructing our fitting procedures either. Nevertheless it could happen that the effect of the nuclear compression will be more visible in theoretical predictions of the spontaneous fission life times, as this effect changes also the fission barrier widths.

Table 1. Differences of the macroscopic energies with compression effect included and not included (in MeV) for a few representative nuclei whose fission barriers are known. As mentioned in the text, the effect of the compressibility is always to lower the barrier. Column 4 contains similar contributions but to the ground-state binding energies. Percentages (column 3) are defined with respect to the experimental barrier heights.

Nucleus	Barrier	[%]	Binding
^{75}Br	−0.93	2.5	−0.064
^{98}Mo	−1.45	3.2	−0.056
^{186}Os	−0.62	2.6	−0.017
^{210}Po	−0.33	1.6	−0.010
^{232}Th	−0.09	1.4	−0.006
^{240}Pu	−0.04	0.7	−0.004
^{252}Cf	−0.02	0.4	−0.002

4. Summary and Conclusions

The present study can be summarized as follows:

1) Taking into account the deformation dependence of the congruence energy significantly approaches the theoretical LSD-model barrier-heights to the experimental data in the case of the light isotopes while the fission barriers for heavy nuclei remain nearly unchanged and agree well with experiment.

2) The effect of the compression energy on the ground states masses and the fission barrier heights is comparable or smaller to the prediction accuracy of the macroscopic-microscopic models, and consequently:

3) It seems that the much higher precision and/or other observables will be needed that could possibly allow conclusions about the compression energy based on the model studied in this paper.

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