Nuclear masses and fission barriers within the isospin-square liquid drop model

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New liquid drop model with the isospin-square dependence of the volume and surface energy terms is applied to reproduce experimentally known masses of nuclei with number of protons and neutrons larger or equal to twenty. The ground-state microscopic energy corrections are taken into account. In spite of the fact that the model contains only six adjustable parameters, the quality of mass reproduction is good, and it is comparable with other contemporary mass models. Also, the fission barrier heights of actinide nuclei evaluated using the topographical theorem of Myers and Świątecki are close to the data.

KEYWORDS: mac-mic model, nuclear masses, fission barrier heights, scission point properties

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I. INTRODUCTION

The liquid-drop (LD) model is one of the oldest nuclear theories. Von Weizsaecker first proposed it [1] 1935. His spherical LD model has reproduced with a reasonable accuracy all measured at that time atomic masses. Four years later, Meitner and Frisch [2] have added deformation degrees of freedom to the LD model to explain the fission phenomenon discovered by Hahn and Strassmann when bombarding the metallic uranium with neutrons [3]. Also in 1939, Bohr and Wheeler proposed this new phenomenon's first theory by expanding the deformed nuclear liquid drop surface in a series of Legendre polynomials [4].

A modern version of the LD model was proposed in 1966 by Myers and Świątecki [5]. They have shown that the LD energy enriched by the shell and pairing effects can describe well the binding energies and quadrupole moments of known nuclei and gives a reasonable description of the fission-barrier height of heavy nuclei (see also [6]). Unfortunately, neither the Myers and Świątecki LD formula nor its refined version called the droplet model could adequately reproduce the barrier heights of medium-heavy and lighter nuclei [7]. In addition, it was shown by von Groote and Hilf [8] that a further correction to the LD model, namely the curvature term, did not change much in this respect. Due to these results further development of the nuclear LD model was stopped in practice for more than three decades. Other much more complicated models like the droplet, Yukawa-folded (YF), Yukawa-plus-Exponential (YpE), or Finite-Range Droplet Models (FRDM) have been used to obtain within the so-called macroroscopic-microscopic (mac-mic) approximation [5] of the binding energies and the fission barrier heights (for overview look, e.g., Ref. [9]).

Twenty years ago, it was shown in Ref. [10] that the original model of Myers and Świątecki with an additional term containing the curvature energy can simultaneously describe the experimental binding energies of all known at that time isotopes as well as the fission barrier heights. One has to stress that this Lublin-Strasbourg-Drop (LSD) model has reproduced the data with better or comparable accuracy than any other *more advanced* theories containing even more adjustable parameters (e.g., Refs.[11, 12]). In the following years, some other parametrizations of the nuclear liquid-drop formula were studied (see, e.g., [13–15]). Unfortunately, the fission-barrier heights estimated using these models are pretty far from the experimental or estimated ones [21].

In the present paper, we will follow the idea of Moretto et al. [15] and use the quadratic in isospin dependence of the nuclear part of the binding energy in the LD formula. Namely, contrary to Moretto, we allow a different isospin-square dependence of the volume and surface terms here. Such extension with respect to the version (i) of the Moretto et al. LD model [15] allows to reproduce much better the experimental masses from the last mass-table [22]. We have used the microscopic energy correction evaluated by Möller et al. [23] to perform the mass fit.

II. THEORETICAL MODEL

A typical nuclear LD formula consists of volume, surface, and Coulomb energy terms:

$$E_{\rm LD} = E_{\rm vol} + E_{\rm sur} \cdot B_{\rm sur}({\rm def}) + E_{\rm Coul} \cdot B_{\rm Coul}({\rm def}) \; . \quad (1)$$

Only the first term is deformation-independent since one assumes that the volume of the nucleus is conserved, while the other terms change with deformation. One has to evaluate their variance assuming some parametrization of the shape of the deformed nuclei. The geometrical, deformation-dependent factors $B_{\rm sur}$ and $B_{\rm Coul}$ have to be evaluated for a given shape parametrization of the deformed nucleus (see, e.g., [16]).

We assume the following isospin-square dependent liquid-drop (ISLD) formula for the energy of a spherical

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nucleus (see also Ref. [15]):

$$
\begin{aligned}
E_{\mathrm{ISLD}}(Z,A) = \; & -a_{\mathrm{vol}} A \cdot \left(1 - 4\kappa_{\mathrm{vol}} \frac{T(T+1)}{A^2}\right) \\
& + a_{\mathrm{sur}} A^{2/3} \cdot \left(1 - 4\kappa_{\mathrm{sur}} \frac{T(T+1)}{A^2}\right) \\
& + \frac{3}{5} e^2 \frac{Z(Z-1)}{A^{1/3}} + E_{\mathrm{odd}}(Z,A) \\
& - \frac{3}{4} e^2 \left(\frac{3}{2\pi}\right)^{2/3} \frac{Z^{4/3}}{r_0 A^{1/3}} \; .
\end{aligned} \tag{2}
$$

Here, Z and A are a nucleus's charge and mass numbers, and $e^2 = 1.43996518\,\mathrm{MeV \cdot fm}$ is the elementary charge square. Here, the volume and the surface part of the binding energies are dependent on the square of the isospin of nucleus $T(T+1)$, which is equal to $T = |T_z| = |N - Z|/2$, where $N = A = Z$ is the neutron number. It is easy to show that

$$
4T(T+1) = |N-Z|(|N-Z|+2)
$$

while in typical LD model were $|N-Z|^2$ present. The odd-even energy E_{odd} is assumed in the following form:

$$
E_{\mathrm{odd}}(Z,A) = \begin{cases} 2\Delta & \text{for Z and N = A} - \text{Z odd} \; , \\ \Delta & \text{for Z or N odd} \; , \\ 0 & \text{for Z and N even} \; . \end{cases} \tag{3}
$$

The last term in Eq. (2) describes the Coulomb exchange energy [24].

Note that the linear in isospin term in the ISLD model (2) corresponds to the Wigner (or congruence) energy present in typical LD-like models (confer, e.g., [5, 12]). In addition, in the ISLD model, the deformation dependence of this linear in $|N - Z|$ is well defined, whereas, in Ref. [12], one has to add an additional phenomenological deformation dependence in order to obtain a doubling of the congruence at the scission point, when two fission fragment nuclei are born. The only free, i.e., adjustable, parameters of the ISLD model are: a_{vol}, κ_{vol}, a_{sur}, κ_{sur}, r_0, and Δ.

The following equation gives the mass of an atomic nucleus:

$$
\begin{aligned}
M_{\mathrm{th}}(Z,A) & = Z \cdot M_{\mathrm{H}} + N \cdot M_{\mathrm{n}} + E_{\mathrm{ISLD}} + E_{\mathrm{micr}} \\
& - 0.00001433\, Z^{2.39} \; ,
\end{aligned} \tag{4}
$$

where M_{H}=7.289034 MeV and M_{n}=8.071431 MeV are the hydrogen and neutron masses measured with respect to the mass unit. The microscopic energy correction originates from the shell and pairing effects. It is equal to the difference between the ground-state energy of the nucleus and its spherical macroscopic energy. The last term approximates the shell energy of electrons.

The Fourier-over-Spheroid (FoS) shape parametrization [17, 18] has been shown to reproduce nuclear shapes very close to the *optimal shapes* obtained by the Strutinsky variational procedure [19] and allows to evaluate precisely the liquid drop energy at the saddle point. Knowing this energy, one can estimate the fission barrier height (V_{sadd}) with the help of the Myers and Świątecki topographical theorem [12]

$$
V_{\mathrm{sadd}} = M_{\mathrm{sadd}}^{\mathrm{mac}} - M_{\mathrm{exp}}(\mathrm{g.s.}) \; , \tag{5}
$$

where $M_{\mathrm{sadd}}^{\mathrm{mac}}$ is the macroscopic mass at the saddle point and $M_{\mathrm{exp}}(\mathrm{g.s.})$ is the ground-state experimental mass. The argument of Świątecki in favor of Eq. (5) was that the shell, or better to say microscopic energy corrections at the saddle-point, are small as the fissioning system, tries to avoid hills and holes on its way to fission. Of course, such argumentation is only valid when one discusses the energy of the highest saddle point, not the deformation of the nucleus at the saddle point. It was shown in Ref. [20] that the above rough approximation reproduces fairly well the experimental fission barrier heights.

III. NUCLEAR MASSES IN DIFFERENT MACROSCOPIC-MICROSCOPIC MODELS

In the last issue of the atomics mass table [22], there are 2259 measured and 906 estimated masses of isotopes with $Z, N \geq 20$ having the experimental error smaller than 1.5 MeV. All these masses are taken to find the best set of six adjustable parameters of our ISLD model (2). The mean square deviation of theoretical estimates and the experimental masses is minimized to obtain the best set of parameters. The microscopic energy E_{micr} from the Möller et al. mass-table [23] were used when evaluating the masses of isotopes using Eq. (4). Two parameter sets are found: one (a) corresponding to 2259 measured masses and the second one (b) obtained using 3165 measured and estimated masses. The r.m.s. deviation, which is a measure of the fit quality, is taken in the following form:

$$
\sigma = \frac{1}{n} \sum_{i=1}^{n} (M_{\mathrm{th}} - M_{\mathrm{exp}})^2 \; , \tag{6}
$$

where i runs over all isotopes taken into account. We have also evaluated σ for three traditional models: Thomas-Fermi (TF) of Myers and Świątecki [12], LSD of Pomorski and Dudek [10], FRDM of Möller et al. [23].

The results are presented in Table I, where n corresponds to the number of nuclei with the measured masses (1st raw) and those 3165 nuclei having measured masses or derived not from purely experimental data and systematics (2nd raw), denoted by # sign in the mass-table [22]. Surprisingly, the 28-year-old Thomas-Fermi model predicts these 906 additional masses better than the FRDM. Also, the LSD model made in 2003 describes both experimental data and all experimental and estimated data very well, proving its good predictive power. It is seen in Table I that the ISLD model with only six adjustable parameters fitted to the experimental data for 2259 isotopes (a) reproduces the isotope masses with even better quality than the FRDM from which the microscopic energy

TABLE I: Root mean square deviations (in MeV) of the experimental masses [22] and the theoretical ones evaluated in different models.

n	TF	LSD	FRDM	ISLD (a)	ISLD (b)
2259	0.669	0.523	0.536	**0.532**	0.638
3165	0.874	0.817	0.956	0.939	**0.760**

corrections are taken. Of course, the r.m.s. deviation of the theoretical and measured masses grows when one makes the fit to all 3165 masses. So, an additional fit (b) of the ISLD parameters was performed when all 3165 isotope masses were considered.

A question appears, which set of the ISLD parameters should be used? The one fitted to the experimental masses only (a) or that adjusted to all experimental and estimated masses (b). Answering this question, one has to note that more than half of the isotopic masses of heavy nuclei with mass-number $A \geq 220$ listed in the mass table [22] corresponds to the estimated, not the measured data. In addition, the pure experimental masses are only less than 10% of the data for the super-heavy nuclei (SHN) with $Z \geq 104$. So, the ISLD parameters listed in Tab. II which corespond to the fit (b) are recommended when describing the properties of the heavy and super-heavy nuclei.

TABLE II: The parameter set of the ISLD (2) model fitted to the experimental and derived from systematics masses (case (b) in Tab. I).

a_{vol}	κ_{vol}	a_{sur}	κ_{sur}	r_0	Δ
MeV	-	MeV	-	fm	MeV
-15.48409	1.8778	17.58207	2.2667	1.21589	11.62

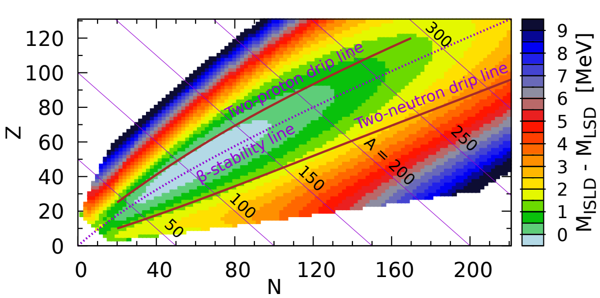

FIG. 1: Difference of the atomic mass estimates obtained using the ISLD (b) and the LSD [10] models.

One has to mention here that we have also performed mass fits by using a similar as (2) LD formula but with the curvature term (proportional to $A^{1/3}$) and the Coulomb redistribution terms ($\sim Z^2/A$). However, adding such two terms to the ISLD formula almost did not change the r.m.s. deviation from the data.

It is well known that the nuclear masses predictions for nuclei close to the β-stability line obtained within different macroscopic models are close. Significant differences between the models may appear when one goes toward the proton or neutron drip lines. This effect is illustrated in Fig. 1, where the differences between the ISLD (b) and LSD mass estimates of all bound systems are shown as a function of neutron (N) and proton (Z) numbers. It is seen that the deferences do not exceed the range (-0.5, 0.5) MeV for isotopes with $A \leq 220$ laying between the two-proton drip and β-stability lines. Also, both estimates are close to each other for neutron reach isotopes close to the β-stability line. In the region of super-heavy nuclei and for isotopes close to the two-neutron drip line, the ISLD masses are even 1.5 MeV larger than the LSD ones. Differences in the mass estimates may be significant for the prediction of the astrophysical r-process or stability and decay of the SHN.

IV. POTENTIAL ENERGY SURFACES AND FISSION BARRIER HEIGHTS

The LSD and ISLD macroscopic energy surfaces of ^{250}Cf are compared in Fig. 2. We have used here the FoS shape parametrization [18]. One has assumed here that the macroscopic energy of a spherical nucleus ($c = 1$, $a_4 = 0$) is zero. It is seen that the surfaces obtained in both models are close to each other, and only tiny differences can be noticed. Namely, the ISLD fission valley (top row) is slightly deeper and corresponds to more elongated shapes than the LSD one. The bottom of the LSD valley around the scission configuration (bottom raw) is located at the elongation $c = 2.62$. It is located around 4 MeV above the ISLD exit from the valley which appears at $c = 2.70$. Such differences in energy and elongation of the nucleus in the macroscopic scission point may have some influence on the total kinetic energy (TKE) of the fission fragments. On the other hand, the stiffnesses of LSD and ISLD potentials with respect to the fission fragment mass asymmetry (A_h) (see the maps in the bottom raw) are very close to each other. The saddle points in both (c, a_4) maps correspond to almost the same energy ($E_{\mathrm{sadd}} \approx 1.3$ MeV and are located around the deformation $c \approx 1.35$ and $a_4 \approx 0.06$.

Such macroscopic saddle-point energies will be used in the following to estimate the fission barrier heights of the actinide nuclei by the topographical theorem of Myers and Świątecki (5).

The fission barrier heights estimated using Eq. (5) and the ISLD and the LSD parameters are compared in Fig. 3 with the experimental data taken from Refs. [25, 26] as well as with the theoretical estimates of the highest fission

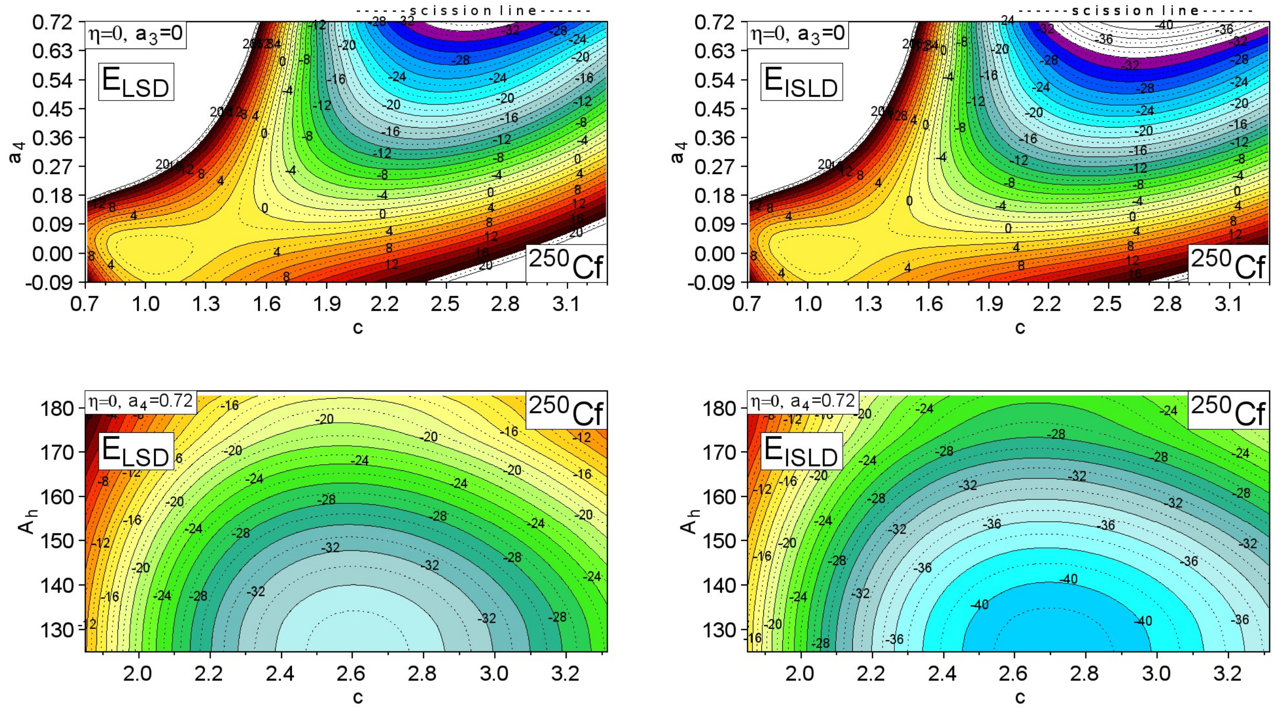

FIG. 2: Macroscopic energy surfaces of ^{250}Cf on the (c, a_4) plane (top) and around the scission configuration (bottom) are evaluated using the LSD (l.h.s) c and ISLD(r.h.s.) formulae. Here c is the elongation of the nucleus, a_4 is related to the neck size, and $\mathrm{A_h}$ is the heavy fission fragment mass number [18].

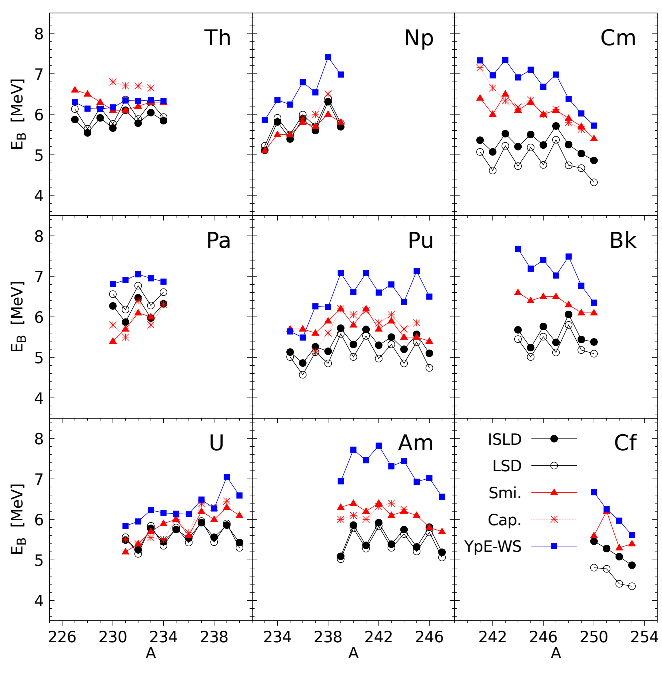

FIG. 3: Fission barrier heights evaluated with the ISLD set of parameters are compared with the empirical/experimental data taken from Ref. [25] (triangles) and [26] (stars) and with the theoretical values (squares) obtained within the mac-mic model in Ref. [27].

barrier made in Ref. [27]. The experimental, or better to say *empirical*, fission barrier heights come mainly from analysis of the fission cross-section energy dependence and fissionability of nuclei, supplemented by data obtained from analysis of the excitation functions of spontaneously fissioning isomers and the group of strong resonances in the sub-barrier fission cross-section [25, 26]. The theoretical barrier heights tabulated in Ref. [27] were evaluated within the 7D mac-mic model with the YpE macroscopic energy part and the microscopic energy evaluated using the Woods-Saxon (WS) single-particle potential.

As one can see, the fission barrier heights obtained using the Myers and Świątecki topographical theorem and the LSD and ISLD models underestimate, in most cases, the experimental barrier heights while those of Ref. [27] are, as a rule, larger than the experimental values. One can expect that the fission barrier evaluated in similar as in Ref. [27] but with the ISLD macroscopic part of the energy will be closer to the data as the topographical theorem says that the effect of the microscopic energy part at the fission saddle is small but not equal to zero.

V. CONCLUSIONS

We have shown that the new liquid drop mass formula with the asymmetry term proportional to the isospin square (ISLD) describes the presently known experimental and estimates masses well. One has to stress here that the ISLD formula contains only six adjustable parameters. The other models contain more free parameters, e.g., the 21 years old LSD mass formula [10], which reproduces the binding energies even better than the FRDM theory [23], possesses eight directly fitted parameters and five others (in the congruence/Wigner and odd-even terms) taken from the adjustments made in Ref. [11]. In this place, it is good to remember that microscopic models, which typically have up to 14 parameters in the interactions, can reproduce 2149 experimental masses with the r.m.s. deviation equal to 0.798 MeV [28].

It was also shown that both ISLD and LSD models describe well the fission barrier heights of the heavy nuclei. The ISLD model predicts slightly larger atomic masses than the LSD one in the super-heavy region of nuclei and for neutron-rich isotopes close to the neutron drip line. This difference in the mass estimates could be significant for SHN physics, and it can influence the nuclear r-process probabilities, which is very important in astrophysical theories. Also, the ISLD model predicts more elongated shape of fissioning nuclei at scission configuration than the LSD formula. This effect can influence on estimates of the fission fragment TKE and their charge equilibration (confer Ref. [29].

We plan to perform extended dynamical calculations like those made in Refs. [18, 29–32] but use the new ISLD formula when evaluating the potential energy surfaces of fissioning nuclei.

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