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Fission properties of Po isotopes in different macroscopic–microscopic models

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Received 15 November 2014, revised 5 February 2015
Accepted for publication 25 February 2015
Published 29 October 2015

Abstract
Fission-barrier heights of nuclei in the Po isotopic chain are investigated in several macroscopic–microscopic models. Using the Yukawa-folded single-particle potential, the Lublin–Strasbourg drop (LSD) model, the Strutinsky shell-correction method to yield the shell corrections and the BCS theory for the pairing contributions, fission-barrier heights are calculated and found in quite good agreement with the experimental data. This turns out, however, to be only the case when the underlying macroscopic, liquid-drop (LD) type, theory is well chosen. Together with the LSD approach, different LD parametrizations proposed by Moretto et al are tested. Four deformation parameters describing respectively elongation, neck-formation, reflectional-asymmetric, and non-axiality of the nuclear shape thus defining the so called modified Funny Hills shape parametrization are used in the calculation. The present study clearly demonstrates that nuclear fission-barrier heights constitute a challenging and selective tool to discern between such different macroscopic approaches.

Keywords: macroscopic–microscopic model, deformation energies, fission process, nuclear shape parametrization

(Some figures may appear in colour only in the online journal)

1. Introduction

Recent experimental studies [1–4], and in particular the discovery of an asymmetric splitting in the low-energy fission of $^{180\text{Hg}}$ clearly show that the competition between predominantly symmetric and asymmetric fission depends on both the atomic number $Z$ (or the fissility) and the $N/Z$ ratio of the fissioning system. To further study these dependences, the polonium ($Z = 84$) isotopic chain, situated mid-way between mercury and the actinide region as such, seems to us of particular interest. In addition, while actinide low-energy fission is primarily determined by the microscopic shell effects in the nascent fragments at large elongation, the mass partition results from a more subtle interplay between the macroscopic and microscopic contributions to the total energy in the considered region. In order to be able to make reliable predictions on the nature of the fission process (symmetric versus asymmetric) it seems of capital interest to rely on a nuclear model that is able to produce a very precise description of nuclear deformation energies. We have therefore investigated the deformation properties along the Po isotopic chain in several macroscopic–microscopic models, using, together with different liquid-drop (LD) models, such as the Lublin–Strasbourg drop (LSD) model [5], different LD type parametrizations recently proposed by Moretto and co-workers [6], as well as by Royer [7] and finally the LD model proposed by Wang [8, 9], the Yukawa-folded single-particle potential [10], together with the Strutinsky shell-correction method [11] and the BCS theory [12] to yield the shell and pairing contributions. It turns out that one is able to generate fission-barrier heights that are in a quite good agreement with the experimental data, as long as the underlying macroscopic, LD type, theory is well chosen. Four deformation parameters describing, respectively, the elongation, neck-formation, reflectional-asymmetric, and non-axiality of the nuclear shape are used in the calculation. This so called modified Funny Hills (MFH) shape parametrization was proposed in [13]. It was also shown that the forms of fissioning nuclei obtained...
using Strutinsky’s theory of optimal LD shapes [15] can be well reproduced within this MFH shape parametrization. We are thus going to show in the present contribution that nuclear fission-barrier heights constitute a challenging and selective tool to discern between such different macroscopic approaches.

2. Macroscopic and microscopic nuclear energy

The total energy of even–even nuclei is determined in our approach on a deformation grid by the macroscopic–microscopic method [12, 16] as the sum of the macroscopic energy \( E_{\text{mac}} \) and the shell and pairing corrections

\[
E_{\text{tot}} = E_{\text{mac}} + E_{\text{shell}} + E_{\text{pair}}.
\]

The microscopic correction to the LD energy consists of the proton shell and pairing energies \( E_{\text{shell}}^{(p)} \) and \( E_{\text{pair}}^{(p)} \) and the corresponding contributions for neutrons:

\[
E_{\text{micr}} = E_{\text{shell}}^{(n)} + E_{\text{pair}}^{(n)}.
\]

The shape of the axially deformed nucleus is described in our MFH shape parametrization in cylindrical coordinates by

\[
\rho_s(z,u) = N(1-u^2)
\]

\[
\times \left[ 1 - Be^{-(1-B)|u-uc^2|} \right].
\]

where \( \rho_s(z,u) \) is the distance of the nuclear surface to the symmetry axis and \( u = (z - z_{sh})/z_0 \). Here the elongation of the shape in \( z \)-direction is given by \( 2z_0 \) and one defines a dimensionless elongation parameter \( c = z_0/R_0 \) with \( R_0 = 1.2 A^{1/3} \) fm. The coordinate \( z_{sh} \) is defined in such a way that the centre of mass of the distribution is located at \( z = 0 \). The normalization \( N \) finally ensures that the density \( \rho_s(z) \) corresponds to the desired (neutron or proton) particle number. The parameters \( c, B \) and \( \alpha \) describe the elongation, neck and reflection asymmetry of the nucleus. Note that the deformation \( c = 1 \) with \( B = 0 \) represents the spherical shape, while the neck parameter \( B = 1 \) corresponds to a scission configuration. We restrict ourselves here to axial symmetric shapes. Triaxial shapes have to be considered at smaller deformations, but play a less important role [17] for very elongated shapes for which the present investigation is carried out (see [13] for the inclusion of the non-axiality degree of freedom).

In order to reduce the numerical effort and eliminate points which, in the deformation plane spanned by the \( c \) and \( B \) parameters, are far from the fission valley, we have introduced the following grid on this plane [13]:

\[
B = 1 - e^c \cos \psi, \quad c = 1 + e^c \sin \psi.
\]

The relation between the new radial coordinates \( \kappa, \psi \) and the \( c, B \) parameters is shown in figure 1 and a small sample of nuclear shapes that can be obtained in this way are displayed in figure 2, with oblate shapes for negative and prolate shapes for positive \( \psi \) values. One can identify the spherical shape that is obtained for \( c = 1 \) and \( \psi = 0 \), in which case the \( \kappa \) parameter corresponds to the neck degree of freedom. For large deformations close to the scission configuration (where \( \psi = \pi/2 \)), it is, however, \( \kappa \) that corresponds to the elongation and \( \psi \) to the neck parameter as can clearly be seen from figure 2.

Figure 1. Relation between the elongation and neck parameters \( c \) and \( B \) of equation (3) and the parameters \( \psi \) and \( \kappa \) introduced through equation (4).

Figure 2. Variety of shapes that are obtained for different \( (\psi, \kappa) \) values in the left–right symmetric (\( \alpha = 0 \), upper part) and asymmetric (\( \alpha = 0.3 \), lower part) case.

Single-particle levels and deformation energies with their macroscopic and microscopic, shell and pairing, contributions for protons and neutrons are calculated in every grid point [14]. The potential energy surfaces in the \( (c, B, \alpha) \) or \( (\psi, \kappa, \alpha) \) deformation space are then analysed around the saddle-point configuration, the location of which might
slightly vary along the Po isotopic chain studied in the present work. The results are presented in the next section.

Such an investigation is carried out for the LSD model [5], but also for the four different Moretto parametrizations of [6]. The LSD model is a LD type parametrization of the macroscopic nuclear energy, including in particular a curvature correction of power $A^{1/3}$ and a deformation dependent congruence-energy term

$$E_B^{\text{LSD}} = a_s \left[ 1 - k_s I \right] A + a_s \left[ 1 - k_s I \right] A^{2/3} B_s + a_s \frac{Z^2}{A^{1/3}} B_{\text{coul}} + a_{cg} \frac{Z^2}{A} + a_{cg} \exp[-4.2 |I|] B_{cg},$$

where the last term is the so-called congruence energy introduced by Myers and Świątecki [18] to take into account the extra binding appearing near the $N = Z$ line (caused essentially by $I = 0$ pairing correlations). Here $I = 1 - 2Z/A$ is the nuclear isospin and the shape functions $B_s$, $B_c$ are obtained as the ratio of the nuclear surface and curvature of the deformed shape relative to the corresponding spherical shape. The Coulomb shape function $B_{\text{coul}}$ is defined in a analogue way and $B_{\text{coul}}$ is specified in [18]. The parameters entering the LSD are given as The LSD approach has been shown, not only to yield an excellent description of nuclear ground-state masses, but to be also able to reproduce fission-barrier heights quite precisely [5].

The LD binding energy proposed by Moretto and co-workers [6] is of the form

$$E_B^{(M)} = \left[ a_A + a_s A^{2/3} + a_c A^{1/3} \right] \times \left[ 1 - k \frac{|J|(|J| + 2)}{A^2} \right] + a_{\text{coul}} \frac{Z(Z - 1)}{A^{2/3}}$$  \hspace{1cm} (6)

with $J = N - Z = IA$, arguing that, when interpreting the asymmetry term as an isospin dependence, the term quadratic in $J$ should be treated as $T^2$, with $T = |N - Z|/2 = |J|/2$ which then leads to a $T^2 = T(T + 1) = |J|(|J| + 2)/4$ dependence. In this way a term linear in $|J|$ is introduced without an additional parameter, as this would be the case with a Wigner term. Let us also note that volume, surface and curvature term carry here the same isospin parameter $k$. The four different parameter sets proposed by Moretto are given in the table 2 where the last column gives the rms deviation of the different Moretto parametrizations from the experimental nuclear masses taking into account the microscopic corrections as determined in [18], values to be compared to a rms deviation of 0.70 obtained in the LSD for a sample of 2766 nuclear masses. For that same sample of nuclei the Moretto parametrizations yield rms deviations of the order of 0.80 in the most favourable case.

The results of these calculations will be shown below together with those obtained with the LSD and the different Moretto parametrizations. There is, of course, no question of displaying the results for all of the 38 LD parametrizations proposed by Royer. These are given in [7] in the form of four tables that selectively test the importance on the quality of the nuclear-mass fit of different terms, like the curvature energy, the different powers of the isospin parameter $I$, the Wigner term of different form and the Coulomb exchange correction term. That is why we have selected among each of the four tables the one parametrization that yields the best rms deviation for the masses. The parameters of these four LD models are given in table 3 below.

The results of these calculations will be shown below together with those obtained with the LSD and the different Moretto parametrizations.

To complete our investigation on the capacity of different LD parametrizations to reproduce at the same time nuclear ground-state masses and fission-barrier heights, we test the parameter set proposed by Wang and collaborators [8, 9], and
The parameters entering the Wang LD model are displayed in table 4 below.

3. Results

Let us start with the deformation energy given in figure 3 for the nucleus $^{212}\text{Po}$ within the LSD model in the $(\psi, \kappa)$ subspace (for axially and left–right symmetric shapes). One identifies the LD saddle point around $(\psi = 1.15, \kappa = -0.20)$ which is almost 9 MeV high, which is in fairly good agreement with the experimental value which can be extracted from figure 5 below to be around 10 MeV.

This barrier is now compared to what is obtained in the Moretto model. We display in figure 4 the deformation energies obtained for the same nucleus $^{212}\text{Po}$ with the four different Moretto parametrizations.

One immediately notices that, with the noteworthy exception of the $M_i$ parametrization, none of the other Moretto LD models is able to give a fair description of the fission energy landscape of the considered $^{212}\text{Po}$ nucleus, by underestimating the barrier height by almost 4.5 MeV for $M_{iv}$ and $M_i$, and by even more for $M_{ii}$.

The question now arises whether the $M_i$ parametrization is also doing a reasonable job when studying the fission barriers of other nuclei. To investigate the isospin behaviour of that LD parametrization, the fission-barrier heights of the Po isotopes between $^{188}\text{Po}$ and $^{212}\text{Po}$ have been determined and are compared with the corresponding barrier heights obtained with the LSD parametrization. This comparison is shown in figure 5.

The analysis of the four here investigated Royer parametrizations gives the following results as shown in figure 6. One notices that whereas the Royer parametrizations extracted from tables 1 and 2 of his paper [7] yield quite reasonable fission barriers for the nucleus $^{212}\text{Po}$ studied here, with barrier heights of respectively 10.15 and 9.3 MeV, the LD parameter set of table 3 (bottom left part of figure 6), which turns out to be the one LD parametrization with the best rms value, yields a much too large barrier height of 15.5 MeV. The barrier corresponding to the LD parametrization of table 4 on the bottom right of figure 6, finally, is with 6.65 MeV much too low.

The very best reproduction of the experimental masses is, according to [8, 9], obtained in the Wang approach with a rms deviation of only 336 keV. It will be therefore interesting to study the deformation dependence of such a LD model. When calculating the expansion coefficients $b_k$, according to equation (10), that define the shape function $B(\text{def})$ to determine the deformation behaviour of the Wang LD model, it turns out, however, that the $b_2$, $b_4$, $b_6$ are all negative for the nucleus $^{212}\text{Po}$ that we would like to study, which simply means that instead of having a minimum at the spherical shape, as it should, the Wang LD model yields a maximum, and such a LD will not produce a stable solution. It turns out, in fact, that one has to go to mass numbers of the order of $A \approx 350$ to find positive $b_2$ values. It is a mystery to us how stable solutions could have been obtained in such a model.
The theoretical macroscopic barriers along the polonium isotopic chain have been compared to the experimental ones, as estimated by Sagaidak and Andreyev (see [21] and references therein). Due to the moderate fissility of polonium nuclei, the determination of the experimental fission barrier can be rather involved. Indeed, to make a Po isotope fission with reasonable (i.e. measurable) probability, some amount of either thermal or rotational excitation energy has to be imparted to the system. This can be most efficiently achieved by means of a heavy-ion fusion reaction. For nuclei with low to moderately fissility, experimental fission barriers are therefore commonly determined by a statistical-model analysis of evaporation-residue and/or fission cross sections, as measured in heavy-ion collisions around the Coulomb barrier. The de-excitation of the compound nucleus is then described with a statistical-model code using standard evaporation theory, taking into account the competition between neutron, proton, alpha and gamma decays, as well as fission. The fission-barrier height is calculated in such a code with an expression of the form:

$$B_f(l) = B_{LD}(l) + \delta E_{\text{exp}},$$

where $B_{LD}(l)$ is the macroscopic fission-barrier height including the influence of rotation, and $\delta E_{\text{exp}}$ is the ground-state shell-correction energy. The macroscopic fission barrier is treated as a free parameter, and extracted from the best description of the experimental cross sections.

It is well admitted that there are a number of uncertain parameters in such a statistical model analysis (see discussion in [21]). Let us simply mention here among others: the nuclear level-density parameter (known as the $a_f/a_n$ ratio), the

Figure 4. As figure 3 but obtained in Moretto’s parametrizations.

Figure 5. Comparison between barrier heights obtained along the Po isotopic chain with the LSD (upper blue) and Moretto $M_i$ (lower red) LD parametrization.
damping of shell effects with temperature, and the influence on angular momentum. With very massive collision partner, there is an additional uncertainty related by the onset of quasi-fission reactions. All these uncertainties taken together, makes the extraction of a so-called experimental fission-barrier height quite model-dependent. One is therefore confronted with an intricate interplay of various poorly known influences, which can lead to more or less un-controlled compensation effects. As a consequence, the experimental fission-barrier heights can often be hardly determined with an accuracy better than about 2 MeV in the polonium region (see e.g. [21]).

For the $n$-deficient $^{188}$Po, the theoretical barrier extracted within the LSD model is about 5 MeV. That compares well with the experimental one which is around 4.5 MeV. A similarly good agreement is obtained along the whole isotopic chain: for the $N = 126$ isotope $^{212}$Po, the theoretical barrier of 9 MeV is close to the 10.5 MeV deduced from the experiment. Due to the model-dependence of the experimental barrier as extracted from heavy-ion fusion reactions, a more precise comparison of theoretical and experimental macroscopic barriers is irrelevant, and the theoretical barrier heights obtained here can be considered reliable. Any more accurate analysis awaits improvements in the ability of extracting precise fission barrier from the experiment.

To get a more complete picture of the capacity of the different LD models to reproduce the experimental fission barriers, we compare in figure 7 the experimental barrier
### Table 3. LD parameters of the Royer LD model.

<table>
<thead>
<tr>
<th></th>
<th>$a_1$</th>
<th>$k_{s1}$</th>
<th>$k_{s2}$</th>
<th>$k_{s3}$</th>
<th>$a_s$</th>
<th>$k_{c1}$</th>
<th>$k_{c2}$</th>
<th>$k_{c3}$</th>
<th>$a_c$</th>
<th>$a_0$</th>
<th>$W_1$</th>
<th>$W_2$</th>
<th>$W_3$</th>
<th>$W_4$</th>
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</thead>
<tbody>
<tr>
<td>$R_1$</td>
<td>-15.5494</td>
<td>0.0</td>
<td>1.8406</td>
<td>0.0</td>
<td>17.9723</td>
<td>0.0</td>
<td>2.077</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>$R_2$</td>
<td>-15.7016</td>
<td>0.1622</td>
<td>1.351</td>
<td>0.0</td>
<td>19.6025</td>
<td>1.223</td>
<td>-1.445</td>
<td>0.0</td>
<td>-15.7016</td>
<td>0.1622</td>
<td>1.351</td>
<td>0.0</td>
<td>19.6025</td>
<td>1.223</td>
</tr>
<tr>
<td>$R_3$</td>
<td>-15.8011</td>
<td>0.0752</td>
<td>1.5133</td>
<td>0.0</td>
<td>20.0578</td>
<td>0.466</td>
<td>-0.223</td>
<td>0.0</td>
<td>-15.8011</td>
<td>0.0752</td>
<td>1.5133</td>
<td>0.0</td>
<td>20.0578</td>
<td>0.466</td>
</tr>
<tr>
<td>$R_4$</td>
<td>-15.1174</td>
<td>0.0</td>
<td>1.7910</td>
<td>0.0</td>
<td>16.6395</td>
<td>0.0</td>
<td>1.803</td>
<td>0.0</td>
<td>-15.1174</td>
<td>0.0</td>
<td>1.7910</td>
<td>0.0</td>
<td>16.6395</td>
<td>0.0</td>
</tr>
</tbody>
</table>
heights with those obtained in the LSD and the Moretto $M_i$ parametrization, the one that yields the best barrier heights. These barrier heights are obtained as the difference between the macroscopic saddle-point energy and the experimental ground-state energy (i.e. including the experimental microscopic energy corrections). Indeed, due to the topographical theorem of Świątecki [22], the total barrier height is just given as this difference. It is precisely this fact of the quasi absence of microscopic energy corrections at the LD saddle that explains why the study of the LD barrier height yields physically relevant information on the fission property of a nucleus (see also [23]).

Figure 7. Comparison of fission-barrier heights obtained in the LSD and the Moretto $M_i$ parametrization with the experiment in the mass range 200–250.

Figure 8. Comparison of location of the proton and neutron drip lines obtained in the LSD and Moretto LD models, as well as the fissility $x = 1$ line, at which the LD fission barrier vanishes.

<table>
<thead>
<tr>
<th>$a_v$</th>
<th>$a_i$</th>
<th>$a_{sym}$</th>
<th>$a_c$</th>
<th>$\kappa$</th>
<th>$\xi$</th>
<th>$a_{pair}$</th>
<th>$a_W$</th>
<th>$\xi_1$</th>
<th>$\xi_2$</th>
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<tr>
<td>−15.5485</td>
<td>17.4663</td>
<td>29.1174</td>
<td>0.7128</td>
<td>1.3437</td>
<td>1.1865</td>
<td>−6.2299</td>
<td>1.0490</td>
<td>0.01037</td>
<td>−0.5071</td>
</tr>
</tbody>
</table>

4. Conclusions

The following conclusions can be drawn from our analysis:

- When performing macroscopic–microscopic calculations to determine the nuclear deformation properties, there is no guarantee that a macroscopic model that yields excellent ground-state masses, will also be able to produce reasonable deformation properties, in particular fission-barrier heights.
- The LSD has been shown to yield not only excellent ground-state properties, in particular masses, but also to produce fission-barrier heights that are in good agreement with the experimental data.
- Out of the four LD-type parametrizations recently proposed by Moretto and co-workers, only $M_i$ gives a fair description of fission-barrier heights, quite close in fact to the ones obtained in the LSD model.
- Other LD type parametrizations like the ones by Royer [7] have also been tested. They yield, at best, barrier heights of the quality of the $M_i$ parametrization discussed here.
- The Wang LD model that, according to [8] yields the best agreement with experimental nuclear masses, turns out to fail to produce any reasonable deformation energy.

One may finally be concerned about the adequacy of the four-dimensional model space chosen in our MFH shape parametrization. The simple fact that the results obtained in this approach are, indeed, extremely close to the ‘optimal LD shapes’ produced by Strutinsky’s variational method [15], seems to indicate that our present version of the MFH shape parametrization must be quite close to physical reality. Even if we believe to have taken into account the most essential degrees of freedom, improvements of our approach are well conceivable. One of them could consist in allowing for different isospin ratios in the two nascent fragments. Tests in such a direction could well be carried out in the future. Doing so, one has, however, to keep in mind to keep the deformation space within reasonable limits to make calculations still tractable.
Acknowledgments

This work has been partly supported by the Polish–French COPIN-IN2P3 collaboration agreement under project number 08-131 and by the Polish National Science Center, grant No. 2013/11/B/ST2/04087.

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