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CONVERGENCE STUDY OF THE FOURIER SHAPE PARAMETRIZATION IN THE VICINITY OF THE SCISSION CONFIGURATION* **

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In a macroscopic–microscopic approach, the Fourier parametrization of deformed shapes is used to describe the deformation-energy landscapes of nuclei in a 6-dimensional deformation space. A special attention is hereby paid to the convergence of this expansion, in particular for nuclear shapes in the vicinity of the scission configuration. It is shown that the Fourier expansion converges very rapidly and that contributions of multipolarity higher that 4 can be safely neglected, even for extreme deformations as they occur close to the scission configuration.

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1. Introduction

Using the macroscopic–microscopic model with the Lublin–Strasbourg Drop (LSD) [1] for the macroscopic part together with the Strutinsky shell-correction method [2] and BCS pairing correlations [3] for the quantum mechanical corrections, where a Yukawa-folded mean-field potential [4, 5] has been used to determine the single-particle energy spectrum for protons and neutrons, the energy of a given nucleus is calculated as a function of the nuclear deformation. In order to exploit in an optimal way all the relavant deformation degrees of freedom, a recently developed Fourier shape

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parametrization [6, 7]

$$\frac{\rho_s^2(z)}{R_0^2} = \sum_{n=1}^{\infty}\left[a_{2n}\cos\left(\frac{(2n-1)\pi}{2}\,\frac{z-z_{\rm sh}}{z_0}\right) + a_{2n+1}\sin\left(\frac{2n\pi}{2}\,\frac{z-z_{\rm sh}}{z_0}\right)\right] \tag{1}$$

has been used. This parametrization has been shown [7–9] to be, indeed, very rapidly converging and able to describe nuclear systems throughout the periodic table. With only 4 deformation parameters, corresponding to elongation, left–right (reflection) asymmetry, neck formation and non-axiality, one is able to describe or predict ground-state properties from the oblate side to the large prolate deformations in the rare-earth region, or more so, in connection with the fission process. It has even been shown that these Fourier shapes are able to predict the mass partitioning in the fission process at low excitation energy, and its evolution with proton and neutron number [7]. This parametrization has been extensively discussed in several of our recent publications [7–9] and shall, therefore, not be further detailed here. Let us simply mention that it can easily be generalized to describe also shapes that break axial symmetry. A crucial point that needs to be emphasized is given by the fact that instead of the Fourier coefficients a_ν defining the shape in Eq. (1), it is far better to define shape coordinates q_ν, determined through the a_ν. These q_ν parameters are defined in such a way that the liquid-drop fission path is given by vanishing q_ν, except for the elongation parameter q_2 which is positive for prolate and negative for oblate shapes ($q_2 = 0$ for a sphere). This analysis changes marginally when quantum effects are included into the picture, but even then, the deformation coordinates q_ν, $\nu \neq 2$ stay small (except possibly of the left–right asymmetry parameter q_3 and the neck (hexadecapole) parameter q_4), which guarantees a very fast convergence of the Fourier shape parametrization [8].

2. Results and discussion

Using the above-defined approach, deformation-energy landscapes can be determined for any nuclear system as a function of the above-introduced shape coordinates q_ν, where special attention will be put on the convergence of the Fourier expansion for large deformations, in particular, close the scission configuration. Since this is precisely the region characterized by the transition from a mono-nuclear to a di-nuclear sytem, special attention needs to be paid to the border line between these two regimes, where the expansion of Eq. (1) will yield negative values, thus defining the scission configuration. To avoid such inconvenience, one should clearly define, as a function of the q_ν shape coordinates, the transition line between simply connected and disconnected shapes. The result of this investigation is

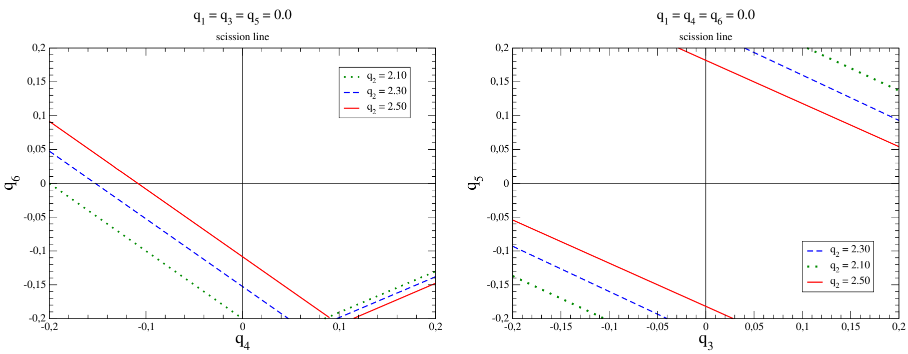

Fig. 1. (Color online) Scission line for axially symmetric systems in the (q_4, q_6) plane (for $q_3 = q_5 = 0$) and the (q_3, q_5) plane (for $q_4 = q_6 = 0$) for different values of the elongation coordinate q_2. Connected shapes are located between lines of the same pattern/color.

shown, for axially symmetric deformations and for different (large) values of the elongation parameter q_2, in Fig. 1 through the border line between connected and disconnected shapes for left–right symmetric deformations ($q_3 = q_5 = 0$) as a function of the (q_4, q_6) parameters and, for left–right asymmetric deformations, as a function of (q_3, q_5) (with $q_4 = q_6 = 0$). The LSD liquid-drop-type energy at such large deformations is shown, again for axially symmetric shapes, as a function of the (q_4, q_6) parameters in Fig. 2. The *forbidden* region of disconnected shapes is clearly visible in the lower left and right corners. To get some feeling about the nuclear shapes that are envolved, we show close to the intersection between allowed and forbidden regions the deformed shapes that are obtained at these points just prior to leaving the allowed region.

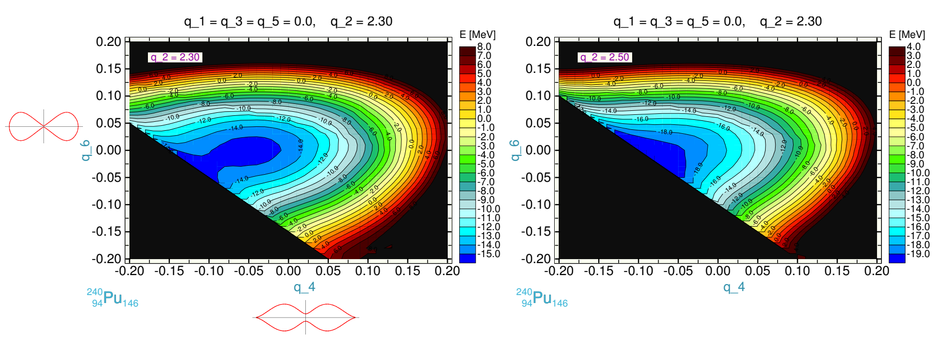

Fig. 2. LSD liquid-drop-type deformation energy for ^{240}Pu in the (q_4, q_6) plane for two different values of the q_2 elongation parameter, $q_2 = 2.3$ (left) and $q_2 = 2.5$ (right). The other deformations coordinates are set to zero. q_1 stands here for the non-axiality parameter (see Refs. [6, 7]).

As a first interesting result, one notices that the minimum energy is always obtained at an essentially vanishing value of q_6. The same, again very favorable result, is found concerning the left–right asymmetry parameter q_5, as demonstrated in Fig. 3 where the deformation-energy landscapes for ^{240}Pu are shown in the (q_3, q_5) plane. While Figs. 2 and 3 are obtained for the liquid-drop part, Fig. 4 shows the same when quantum corrections are included in the calculation.

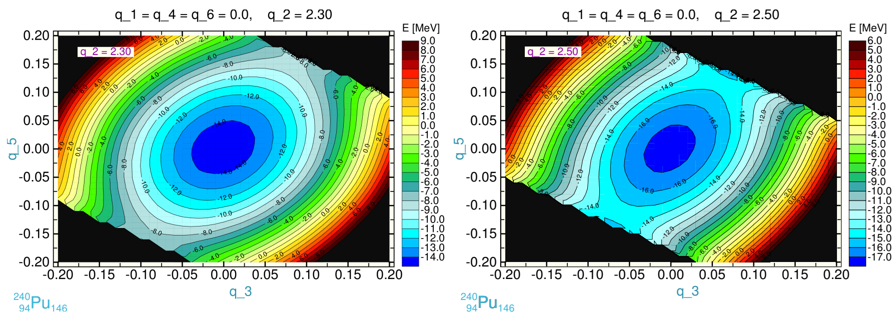

Fig. 3. The same as Fig. 2 for the (q_3, q_5) deformation plane for 2 different values of the elongation parameter, $q_2 = 2.3$ and 2.5. The other deformations coordinates are set to zero.

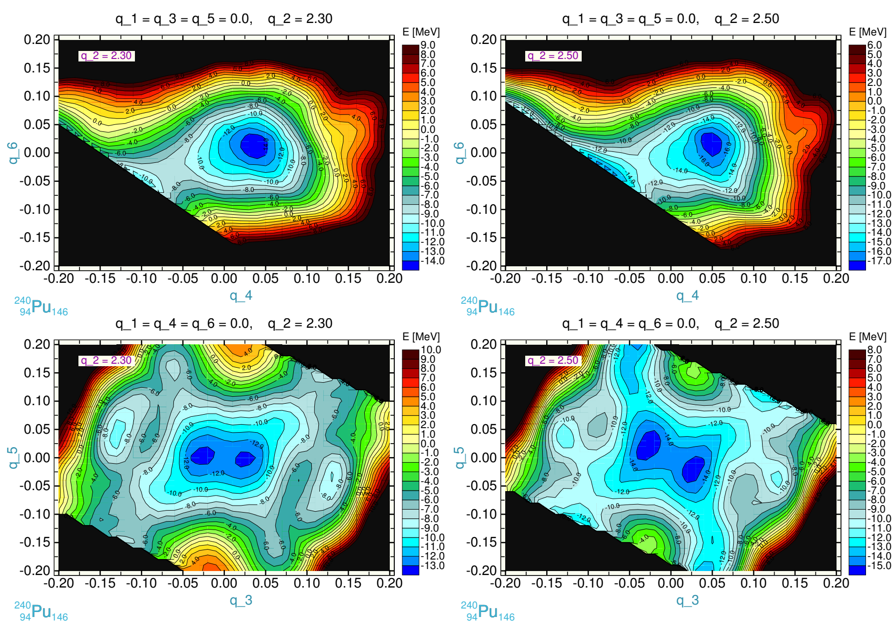

Fig. 4. Deformation energies for ^{240}Pu as Figs. 2 and 3 but now with the inclusion of shell and pairing-correction energies.

From both these figures one concludes again that, even for the extreme deformations considered here (see the shapes sketch in Fig. 2), the higher-order shape coordinates are essentially not coming into play.

One could now argue that for heavy nuclei like ^{240}Pu, where saddle and scission points are well separated, the situation might be different than in lighter nuclei where they are rather close together. We have, therefore, done the same kind of study for ^{202}Hg, but, here again, the location of the minimum-energy points in the (q_3, q_5) and (q_4, q_6) landscapes do practically not change.

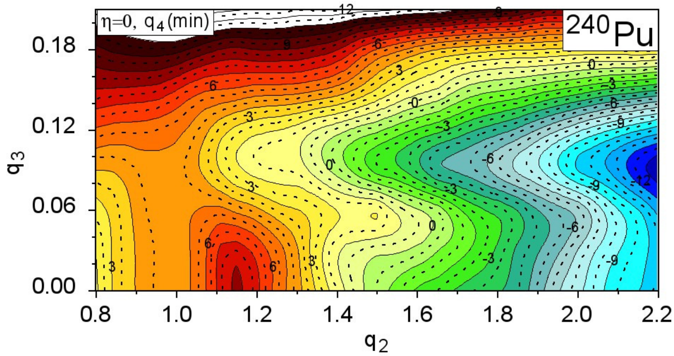

Fig. 5. Total deformation energy for the nucleus ^{240}Pu in the (q_2, q_3) plane, obtained after minimisation with respect to q_4. A symmetric ($q_3 = 0$) and an asymmetric fission valley (at $q_3 \approx 0.09$) are clearly identified.

Up to this point, our systematic study seems to indicate that the higher-oder shape coordinates (beyond q_4) do not play any role and can safely be neglected in the study of the fission process. To confirm our conclusions, let us investigate in some detail the behaviour of the different (left–right symmetric and asymmetric) fission valleys in ^{240}Pu. A left–right asymmetric fission valley is clearly identified corresponding to a q_3 parameter of $q_3 \approx 0.09$.

For a value of the elongation parameter $q_2 = 2.1$, the value of q_4 which minimises the total (quantum) energy is $q_4 = -0.10$. We are, therefore, exploring the energy landscape for these coordinates in the (q_5, q_6) deformation space, as shown in Fig. 6. The left–right symmetric ($q_3 = 0$) fission chanel is found for the same elongation ($q_2 = 2.1$) to correspond to a neck parameter of $q_4 \approx 0.02$. The corresponding (q_5, q_6) landscape is shown in Fig. 7.

From both these figures we conclude that the Fourier shape coordinates that minimize the total energy including quantum corrections are well-approximated by $q_5 = q_6 = 0$. In other words, even for such extreme deformations as those occuring close to the scission instability, neglecting the Fourier shape parameters beyond q_4 turns out to be a very good approximation.

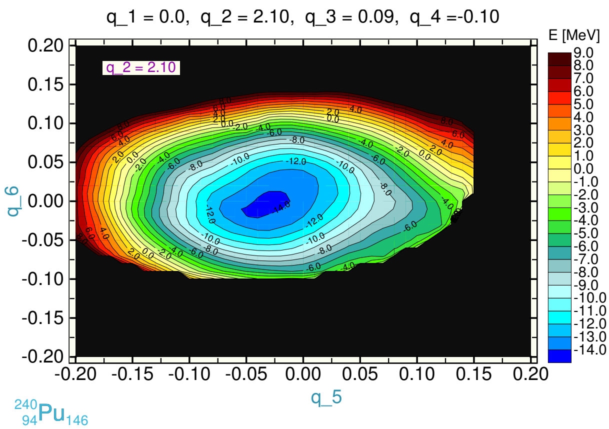

Fig. 6. Energy landscape in the (q_5, q_6) deformation space for the nucleus ^{240}Pu at an elongation defined by $q_2 = 2.1$ and an asymmetry of $q_3 = 0.09$, corresponding to the asymmetric fission chanel identified in Fig. 5.

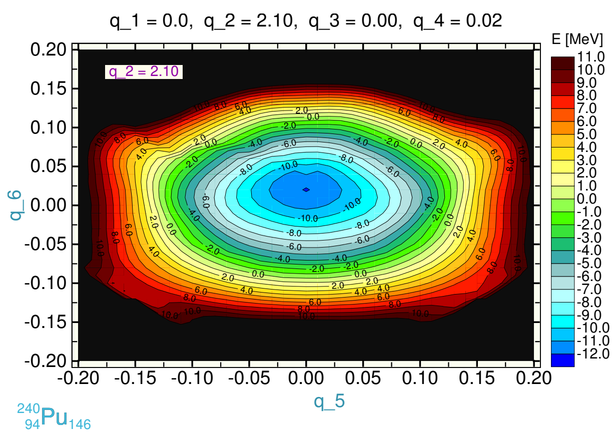

Fig. 7. The same as Fig. 6, but now for the symmetric ($q_3 = 0$) fission chanel at the same elongation.

3. Summary

Using the Lublin–Strasbourg Drop, shown to reproduce nuclear masses and fission barrier heights practically throughout the periodic table, together with Strutinsky and BCS quantal corrections, we have calculated nuclear deformation energies as a function of the deformation coordinates of a Fourier shape parametrization that has now also been extensively tested and proven to be both very flexible and extremely rapidly converging. We have shown that with only 4 deformation parameters corresponding to elongation, left–right asymmetry, neck formation and non-axiality, one is able to account for the deformation from the oblate side up to the very large deformations encountered in the fission process. In the present contribution, we have especially studied the convergence of the Fourier expansion in the immediate vicinity of the scission instability and found that, here again, the above-mentioned 4 deformation coordinates are perfectly sufficient to account for the relevant degrees of freedom in the fission process. This very recomforting result paves the way, as we believe, to carry out extensive calculations of fission dynamics by soving the Langevin equation in a 4-dimensional deformation space. Work along this direction is under way.

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