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2017 Phys. Scr. 92 064006

(http://iopscience.iop.org/1402-4896/92/6/064006)

IOP Publishing | Royal Swedish Academy of Sciences Physica Scripta
Phys. Scr. **92** (2017) 064006 (6pp) https://doi.org/10.1088/1402-4896/aa7002

Fourier expansion of deformed nuclear shapes expressed as the deviation from a spheroid

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Received 12 January 2017, revised 20 April 2017
Accepted for publication 28 April 2017
Published 25 May 2017

Abstract
A Fourier decomposition of nuclear shapes is proposed and shown to be able to cover a very wide range of nuclear deformations up to the scission point. This Fourier shape parametrization is applied to the deviations of a nuclear liquid-drop profile from a spheroidal shape. It is shown that such a shape profile expansion is not only very rapidly converging, but also gives an excellent description of nuclear shapes all along the path to fission. Some examples of the liquid-drop and the macroscopic–microscopic potential energy surfaces in this new shape parametrization are presented and the connection with Bohr (β, γ) deformation parameters is given.

Keywords: shapes of nuclei, fission barrier heights, path to fission, nuclear liquid drop model

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

1. Introduction

An accurate description of the shapes of fissioning nuclei that, at the same time, relies on only a few collective parameters, is one of the most difficult tasks nuclear physicists have been confronted with since the very early days of nuclear physics and the seminal work of Bohr and Wheeler [1] on the theory of nuclear fission. A large variety of nuclear shape parametrisations have been proposed, among which an expansion of the surface of the liquid drop (LD) in a series of spherical harmonics, originally proposed by Lord Rayleigh in the 19th century [2], is still one of the most widely used. Among other, more recent shape parametrizations one needs to quote the so-called quadratic surfaces of revolutions (QSR) by Nix in 1969 [3], intensively explored by Moller *et al* co-workers (see e.g. [4]), the Cassini ovals in the version proposed by Pashkevich from 1971 [5, 6], the so-called funny-hills (FH) shape parametrization introduced by Brack *et al* [7] and its modified version (MFH) (including a Gaussian neck and nonaxiality) from 2004 [8], as well as an expansion of the nuclear surface in a series of Legendre polynomials, due to Trentalange, Koonin and Sierk (TKS) [9].

One of the till nowadays most frequently used parametrization is the expansion due to Lord Rayleigh of the nuclear radius in a series of Legendre polynomials (equation (33) of [2]):

$$R(\theta) = R_0 \sum_{\lambda=0}^{\lambda_{\max}} \beta_\lambda P_\lambda(\cos\theta), \tag{1}$$

where R_0 is the radius of the spherical nucleus having the same volume as the deformed one.

It was shown, however, [8] that this expansion is converging very slowly, and that, at elongations, between saddle and scission point, a very large number of terms (up to β_{14}) is required to correctly describe the nuclear shape and its corresponding LD energy. This implies, however, that one is obliged to handle functions of very large dimension and search for stationary points in a multi-dimensional landscape in order to locate ground state, isomeric states, saddle points, valleys and ridges between them. Up to eight parameters were used in [10] to describe nuclear shapes.

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The QSR, FH or MFH parametrisations, on the other hand, describe nuclear potential energy surfaces rather well with a very limited number of collective variables, but have the fundamental inconvenience that there is no way of controlling their convergence, which is possible, however, by the Lord Rayleigh or the TKS expansion. In what follows, we are going to present a parametrization based on a Fourier expansion of the nuclear surface, which is rapidly converging and which will be shown to describe very well both the ground state and very elongated shapes of the nucleus, close to the scission configuration.

2. Fourier expansion of nuclear shapes

In [11] we have proposed to expand the nuclear shape profile function, written in cylindrical coordinates and presented in figure 1 into a Fourier series by expanding the square distance from the surface to z-axis into a series of sin and cos functions

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

where, as in (1), R_0 is the radius of the corresponding spherical shape, z_0 is half the nuclear elongation and $z_{\rm sh}$ ensures that the nuclear centre of mass is always located at the origin of the coordinate system, i.e. at $z = 0$.

It now turns out that when the nuclear shape becomes more and more elongated the leading-order coefficient a_2 decreases, which is somewhat contrary to our intuition (the corresponding FH parameter c increases with growing elongation). In addition, we have in mind to keep the number of deformation parameters as restricted as we possibly can. That is why we define new parameters q_n in the place of the Fourier coefficients by the following transformation

$$\begin{aligned} q_2 &= a_2^{(0)}/a_2 - a_2/a_2^{(0)}\,,\; q_3 = a_3, \\ q_4 &= a_4 + \sqrt{(q_2/9)^2 + (a_4^{(0)})^2}\,, \\ q_5 &= a_5 - a_3(q_2 - 2)/10, \\ q_6 &= a_6 - \sqrt{(q_2/100)^2 + (a_6^{(0)})^2}\,, \end{aligned} \tag{3}$$

where the $a_n^{(0)}$ correspond to the values of the Fourier coefficients for a spherical shape ($a_2^{(0)} = 1.03205$, $a_4^{(0)} = -0.03822$, and $a_6^{(0)} = 0.00826$). We will show below that already with only 3 deformation parameters q_2, q_3 and q_4 one is able to obtain a very good description of nuclear shapes all along the LD fission path and, in fact, reproduce the shapes and energies obtained by the Strutinsky optimal shapes method [13] with a very good accuracy.

The physical interpretation of the new coordinates is evident: q_2 describes the nuclear elongation, q_3 its left–right asymmetry, and q_4 the neck degree of freedom. Higher order parameters like q_5 and q_6 control the deformation of the nascent fission fragments. In practice it turns out that there is no need to include higher multipolarities, beyond a_6 since the energy difference between the Fourier expansion and the Strutinsky optimal shapes becomes negligibly small. Note that the above proposed Fourier expansion, equations (2) and (3), contains the same number of deformation parameters as the five-dimensional QSR parametrization [3, 4], but contrary to the latter, the Fourier shapes are given by analytical functions with continuous derivatives and, in addition, one can always control the contribution to the energy given by higher order expansion term.

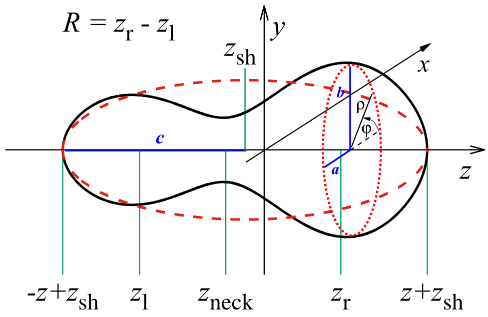

Figure 1. Fourier profile function (solid line) in cylindrical coordinates as compared with a spheroidal shape (dashed line) having the same elongation and volume. For non-axial shapes, an ellipsoidal section (dotted line) is imposed in the z = const plane with half-axis $a(z)$ and $b(z)$. Adapted with permission from [16], Copyright (2017) by the American Physical Society.

Instead of using the Fourier expansion to describe directly the nuclear shape function $\rho_s^2(z)$ as done in (2) and exploited extensively in [16], one can use the same approach to describe the deviation of the shape from a spheroidal form, as presented by the dashed line in figure 1. Such a spheroid is described by the equation

$$\frac{x^2}{A^2} + \frac{y^2}{B^2} + \frac{z^2}{C^2} = 1, \tag{4}$$

where A, B, and C are its main half-axis, assuming in the following that the volume of the spheroid is the same as the one of the spherical nucleus, i.e. $A\,B\,C = R_0^3$. For the axially symmetric case where $A = B$, equation (4) can be rewritten in cylindrical coordinates as

$$\rho_{\rm el}^2(z) = x^2 + y^2 = A^2\left(1 - \frac{z^2}{C^2}\right), \tag{5}$$

where $\rho_{\rm el}$ is the distance of a point on the surface of the spheroid to the z-axis. Note that the C half-axis is the same as the FH elongation parameter c [7].

The deviation of the square distance $\rho_s^2(z)$ from the one of the spheroidal shape can then be expanded into a Fourier series in a similar way as in equation (2):

$$\frac{\rho_s^2(z) - \rho_{\rm el}^2(z)}{R_0^2} = \sum_{n=1}^{\infty}\left[a_{2n}\cos\left(\frac{(2n-1)\pi}{2}\,\frac{z-z_{\rm sh}}{z_0}\right) + a_{2n+1}\sin\left(\frac{2n\pi}{2}\,\frac{z-z_{\rm sh}}{z_0}\right)\right]. \tag{6}$$

Volume conservation and the centre-of-mass condition lead then to the following relations:

$$a_2 = a_4/3 - a_6/5 + a_8/7 - \ldots \tag{7}$$

and

$$z_{\rm sh} = R_0 \frac{3c^2}{2\pi}(-a_3 + a_5/2 - a_7/3 + \ldots). \tag{8}$$

In the axial symmetric case, the shape of a nucleus is then described by the following parameter set: $c, a_3, a_4, a_5, a_6, \ldots$. For reflection symmetric shapes only the parameters c and a_{2n} count.

Non-axial shapes one can describe, in a first approximation, assuming that each cross-section of the nucleus perpendicular to the z-axis has the form of an ellipse with different $a(z)$ and $b(z)$ half-axis. The nonaxiality can then be described by an additional parameter

$$\eta(z) = \frac{b(z) - a(z)}{a(z) + b(z)} \tag{9}$$

and for each z the following relation needs to be fullfield

$$\rho_s^2(z) = a(z)\, b(z), \tag{10}$$

in order to ensures that the volume of axial and nonaxially deformed shape are the same. In equation (11) the nonaxiality parameter η is generally z dependent, which would allow to describe e.g. the so-called *propeller mode* of nascent fission fragments in the region of the scission configuration. In our investigation, we will suppose, however, that η is z independent

$$\eta = \frac{B - A}{A + B}. \tag{11}$$

A large community of nuclear physicists is used to work with the quadrupole axial and non-axial Bohr deformation parameters (β, γ) [14]. That is why we would like to use these in order to describe spheroidal shapes:

$$A = R(\beta, \gamma)\left[1 + \sqrt{\tfrac{5}{4\pi}}\beta\cos(\gamma + \pi/3)\right],$$
$$B = R(\beta, \gamma)\left[1 + \sqrt{\tfrac{5}{4\pi}}\beta\cos(\gamma - \pi/3)\right],$$
$$C = R(\beta, \gamma)\left[1 + \sqrt{\tfrac{5}{4\pi}}\beta\cos(\gamma)\right] \tag{12}$$

where the radius $R(\beta, \gamma)$ is again determined by volume conservation

$$R(\beta, \gamma) = \frac{R_0}{\left[1 - \frac{3}{4}k^2 + \frac{1}{4}k^3\cos(3\gamma)\right]^{1/3}} \tag{13}$$

with $k = \sqrt{\frac{5}{4\pi}}\beta$.

The relation between the (c, η) and the Bohr (β, γ) parameters is displayed in figure 2, where the LD deformation energy in surface-energy units $\Delta E_{\rm LD} = (E_{\rm LD} - E_{\rm LD}^{\rm sph})/E_{\rm surf}^{\rm LD}$ of a nucleus with fissility parameter $x = 0.8$ is shown on the (c, η) plane. Lines of constant β and γ values are given by solid blue lines. Please notice that lines of constant β do not correspond at all to a constant elongation of the nucleus (as given by c) and that their curvature leads to a smaller stiffness of the PES for constant β than for constant c.

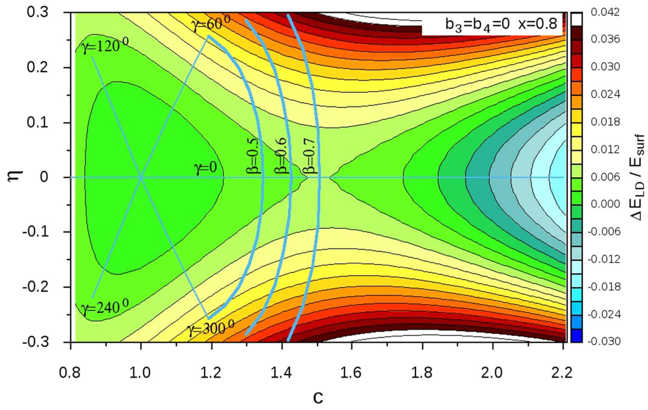

Figure 2. Variation of the liquid drop energy, relative to the spherical shape (in units of the surface energy) in the (c, η) plane for a nucleus with fissility parameter $x = 0.8$. Lines of constant values of the Bohr deformation parameters β and γ are displayed by solid blue lines.

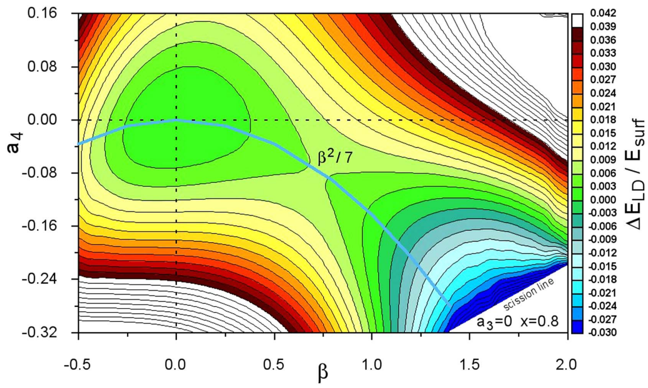

Figure 3. Liquid drop PES in the (β, a_4) plane for a nucleus with fissility parameter $x = 0.8$.

An example of the LD potential energy surface on the (β, a_4) plane is presented in figure 3. The potential energy of an axially symmetric ($\eta = 0$) nucleus with fissility parameter $x = 0.8$ is expressed here in units of the surface energy. The solid blue line $a_4 = \beta^2/7$ corresponds roughly to the minimal energy LD path to fission for the case of a left–right symmetric ($a_3 = 0$) shape. It therefore appears more convenient to use a deformation parameter $b_4 = a_4 - \beta^2/7$ rather than the bare a_4, when studying the PES. The same map as that of figure 3, but in the coordinates (β, b_4) is shown in the upper lhs panel of figure 4. One can see that the line $b_4 = 0$ goes from the spherical equilibrium through the saddle point up to the vicinity of the scission configuration. The role of the a_6 deformation parameter is shown on the upper rhs part of figure 4, where the LD energy is plotted on the (β, a_6) plane. The solid blue line $a_6 = \beta^2/100$ shown in that figure obviously corresponds roughly to the path to fission and the effect of taking the a_6 degree of freedom into account gives only a small modification of the LD fission-barrier height. The effect of the a_5 deformation parameter is also small as can be seen in the (a_3, a_5) plane for the saddle point (lhs) and around the scission configuration (rhs) on the bottom row of figure 4. The line $a_5 = -\beta^2\, a_3/8$ shown on both plots

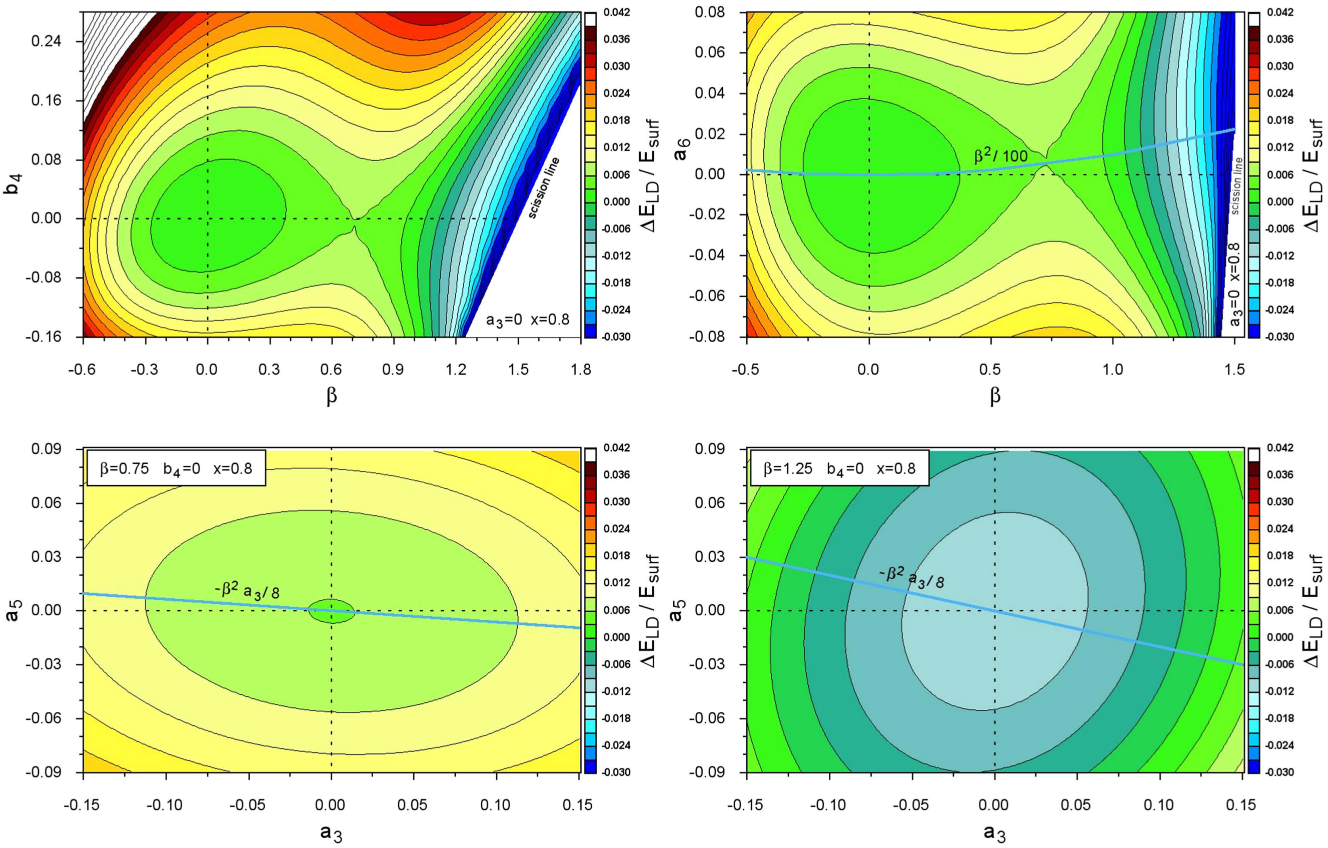

Figure 4. Liquid drop PES relative to the spherical shape (in surface-energy units) for a nucleus with fissility parameter $x = 0.8$, in the (β, b_4) plane (upper lhs), in the (β, a_6) plane for $b_4 = 0$ (upper rhs), as well as in the (a_3, a_5) plane at the saddle point ($\beta = 0.75$, lower lhs) and around the symmetric scission point ($\beta = 1.25$, lower rhs).

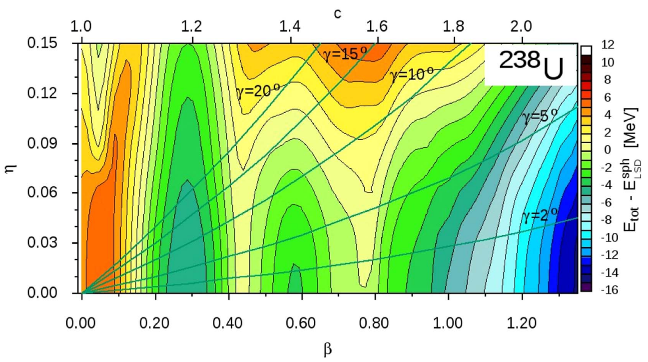

Figure 5. Microscopic–macroscopic potential-energy surface in the (β, η) plane for ^{238}U. Solid blue lines correspond to curves of constant γ.

obviously parametrises rather well the mass asymmetric mode corresponding to the minimal slope of the LD energy.

As a result of the above discussion we propose, similarly to equation (3), the following effective collective coordinates when the Bohr parameter β is used to describe the nuclear deformation

$$b_3 = a_3\,, \quad b_4 = a_4 - \beta^2/7, \quad b_5 = a_5 + \beta^2 a_3/8,$$
$$b_6 = a_6 - \beta^2/100. \tag{14}$$

The advantage of this presentation obviously is that in these new deformation parameters the LD path to fission is now simply given by $b_3 = b_4 = b_5 = b_6 = 0$.

3. Examples of the macroscopic–microscopic potential energy surfaces

For the description of low energy nuclear fission it is essential to take quantum corrections into account. The PES should therefore be evaluated within a fully microscopic model like the Hartree–Fock–Bogolubov theory, or by using a much simpler macroscopic–microscopic approach (see e.g. [15]). The latter has been widely and successfully used to study the properties of nuclei both in the ground state, as well as at large deformations corresponding e.g. to fission isomer states, saddle points or near the scission configuration [4, 10].

An extended calculation within the macroscopic–microscopic model using the Fourier parametrisation (2) of nuclear shapes was recently preformed [12, 16] for nuclei from Pt up to Pu. The macroscopic part of the PES was evaluated using the Lublin–Strasbourg drop (LSD) model [17], while the Yukawa-folded single-particle potential [18] and the Strutinsky shell-correction method [19] with an 8th order curvature correction [20] were used together with the BCS formalism [15] to obtain the microscopic part. An

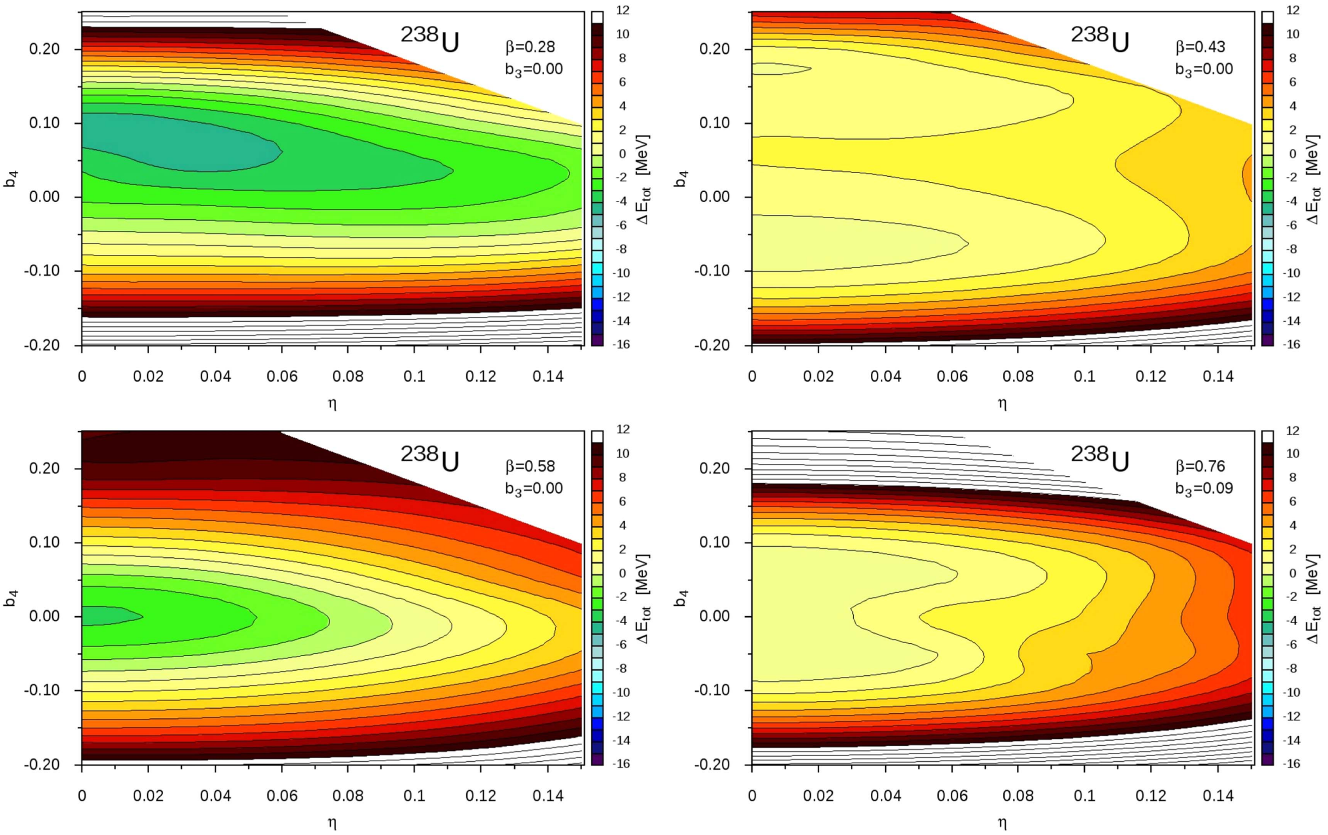

Figure 6. Potential energy surface of ^{238}U on the (η, b_4) plane in the vicinity of the ground state ($\beta = 0.28$, upper lhs map), at the first saddle ($\beta = 0.43$, upper rhs map) and in the bottom raw at the second minimum ($\beta = 0.58$, lhs map) and at the 2nd (asymmetric) saddle point ($\beta = 0.76$, rhs map).

approximate particle-number projection [22, 23] was used when evaluating the pairing energy correction.

In the present contribution we have performed the same kind of calculation for the ^{238}U nucleus, but using the Fourier shape parametrization, equations (6) and (14), for the deviations from a spheroid. That calculation was performed in the 4D deformation parameters space: c, η, b_3 and b_4. The cross sections of the obtained PES are presented in figures 5 and 7 on the (β, η) and the (β, b_3) planes, respectively. The total energy in each deformation point was minimised with respect the two other collective coordinates. The relation between the elongation and nonaxiality parameters (c, η) and the Bohr deformation parameters (β, γ) as described by equation (12) is shown in figure 5 by the blue solid lines. It is seen that the prolate minimum located at $\beta = 0.24$, the first saddle at $\beta = 0.42$ and the second minimum at $\beta = 0.59$ correspond to axial- ($\eta = \gamma = 0$) and reflection-symmetric ($b_3 = 0$) shapes, while in the second saddle at $\beta = 0.76$ the nucleus is reflection asymmetric ($b_3 = 0.09$).

Cross-sections of the PES corresponding to the (η, b_4) plane are presented in figure 6 for ^{238}U in four stationary points: first minimum, first saddle, second minimum and second saddle point. One can clearly see that in all four cases the minimum corresponds to axially symmetric ($\eta = 0$) shapes. It is also visible that the PES around the ground state and both saddle-point configurations is rather soft with

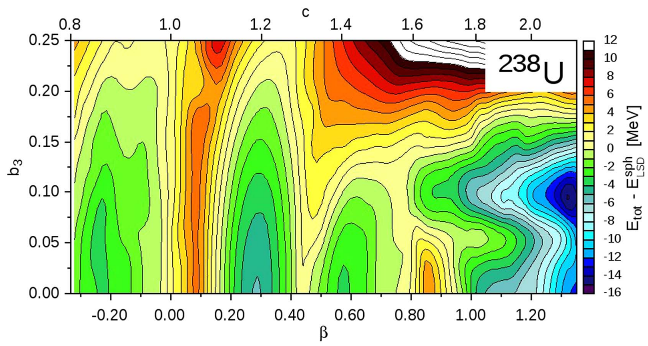

Figure 7. Microscopic–macroscopic potential energy surface in the (β, b_3) plane for ^{238}U.

respect to the nonaxial degree of freedom. No reduction of the first barrier height due to nonaxiallity is observed.

One can wonder why in our calculation the first barrier corresponds to axially symmetric shape while in other models this was not the case. One could think of three possible reasons.

- Different shape parametrisation: in the traditional (β, γ) deformation set for example, the constant β does not corresponds to a constant elongation of a nucleus, as can be seen in figure 2. Note, when one draws a circle in figure 5 with radius $\beta = 0.43$ and the origin at $\beta = \eta = 0$ one can see that the circle crosses layers which correspond to lower energies than the saddle-point energy. In addition, in a majority microscopic–macroscopic calculations, the γ deformation does not correspond directly to a nonaxial quadrupole deformation but it has some admixture of nonaxial hexadecapole deformations in order to preserve the Bohr symmetry (see e.g. [21]).

- Differences in the macroscopic model: we have used in our calculations the LSD macroscopic energy which is not so soft with respect deformations perpendicular to the fission mode as e.g. the Yukawa+exponential energy [17].
- Pairing interaction treatment: we are solving the BCS equations using the GCM+GOA model described in [22] what corresponds to an approximate particle-number projection while in a majority of papers the Lipkin–Nogami method is used.

It turns out that the first saddle point is located at about 5.8 MeV above the ground state minimum. The shape isomeric minimum lies around 2 MeV above the ground state, while the second saddle is about 5.4 MeV above the g.s. These data are, indeed, in quite close agreement with the experiment [24], and this in spite of the fact that none of the parameters entering our calculation was adjusted to reproduce fission barrier heights. The asymmetric fission valley is located below the symmetric one and ends at $\beta \approx 1.35$ and $b_3 = 0.09$ which corresponds to a mass for the heavier fragment of about 140, just as it is seen in the experiment.

Conclusions and perspectives

Our new Fourier expansion of nuclear shapes has been applied to the deviation of the shape from the one of a corresponding spheroid, instead of describing that shape directly. It has been shown that such an expansion, relying on only four deformation parameters, corresponding to elongation, left–right asymmetry, neck degree of freedom and nonaxiality, is very rapidly converging, in particular when a set of effective deformation parameters as given by equation (14) is introduced. The nuclear energies obtained in this way turn out to be, indeed, very close to the experimental data, as has been demonstrated by calculating the energy surface of the actinide nucleus ^{238}U in the framework of the macroscopic–microscopic approach with the LSD model for the liquid-drop part and quantum corrections obtained through a Yukawa-folded mean field potential by the Strutinsky shell-correction method and the BCS theory with a monopole pairing interaction. Further, more extensive investigations, including nuclei in the super-heavy region are on our agenda.

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 Centre, grant No. 2013/11/B/ST2/04087.

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