UNIVERSAL, LOW-DIMENSIONAL SHAPE PARAMETRIZATION OF FISSIONING NUCLEI*

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A new parametrization of nuclear shapes is proposed as a Fourier series of the square of the distance from the symmetry axis to the surface of the nucleus. It is shown that using the three lowest terms of such an expansion is sufficient to obtain a rather good reproduction of the form of the liquid-drop fission barrier. Taking into account higher order terms of the rapidly converging Fourier series increases the precision of the estimates of both macroscopic and microscopic parts of the total nuclear binding energy.

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1. Introduction

A precise but low-dimensional description of nuclear shapes, in particular in connection with fission, is one of the most demanding tasks nuclear physicists have been confronted with since the first paper of Bohr and Wheeler on the fission process [1]. It turns out that the traditional expansion of the nuclear surface in spherical harmonics, proposed by Lord Rayleigh in the $20^{\rm th}$ century, is converging rather slowly. It has, indeed, been shown in Ref. [2] that one needs at least the 7 lowest-order terms of such an expansion in order to obtain an accurate profile of a left–right symmetric liquid-drop fission

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barrier, to describe the nuclear shape from the ground state, through the saddle up to the scission point. A reasonably good description of the fission barrier is obtained using the Funny-Hills (FH) shape parametrization [3] or its improved version known as the Modified Funny-Hills (MFH) shapes [2]. It is, however, difficult to get an estimate of the accuracy of the calculated energies of fissioning nuclei that can be obtained in these two parametrizations. Using a rather similar description, expanding the square distance $\rho_s^2(z)$ from a surface point to the symmetry z axis in terms of Legendre polynomials as proposed by Trentalange, Koonin and Sierk (TKS) [4], such an estimate on the accuracy can be given by simply carrying the expansion to higher orders. The TKS expansion is, however, difficult to handle since the obvious condition $\rho_s^2(z) > 0$ imposes strong limitations onto the involved deformation parameters [2]. Other often quite powerful parametrizations of the nuclear shape exist of course and can be found *e.g.* in Refs. [5, 6]. An alternative expansion of $\rho_s^2(z)$ into a Fourier series, as proposed below, seems be rapidly converging and easier to handle.

2. Fourier expansion of deformed shapes

The profile function of any nuclear shape is expanded in a Fourier series

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

where $\rho_s(z)$ is the distance from a point on the surface at coordinate z (see Fig. 1) to the symmetry axis (z axis) and R_0 the radius of the corresponding spherical shape having the same volume. The extension of the shape along the symmetry axis is $2\,z_0$ with left and right ends located at $z_{\rm min} = z_{\rm sh} - z_0$ and $z_{\rm max} = z_{\rm sh} + z_0$, where ρ_s vanishes, a condition which is automatically satisfied by (1). The shift coordinate $z_{\rm sh}$ is chosen such that the centre of the nuclear shape is always located at the origin of the coordinate system. One

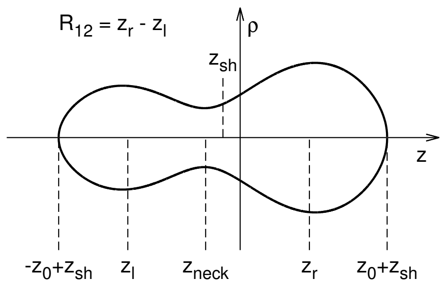

Fig. 1. Nuclear shape parametrization in cylindrical coordinates.

introduces through $z_0 = cR_0$ an elongation parameter c that is equal to unity for the sphere, smaller than one for oblate and larger than one for prolate deformations. The parameters a_2, a_3, a_4 describe respectively quadrupole, octupole and hexadecapole deformations, or better to say, elongation, reflection asymmetry and neck degree of freedom.

Due to the high incompressibility of nuclear mater, one assumes that the volume of a deformed nucleus is the same as the one of spherical shape which yields the following relation between the elongation parameter c and all even coefficients a_n

$$\frac{\pi}{3c} = \sum_{n=1}^{\infty} (-1)^{n-1} \frac{a_{2n}}{2n-1} \,. \tag{2}$$

This relation allows to evaluate the coefficient a_2 as a function of the elongation c and the higher order coefficients a_{2n}. The spherical shape corresponding to $c = 1$ and $\rho(z_{\rm sh})/R_0 = 1$ leads to the following values of the expansion coefficients: $a_2 = 1.03205$, $a_4 = -0.03822$, ...

In the case of symmetric fission, $z_{\rm sh} = 0$ and the geometrical scission configuration is located at $z = 0$ which implies (see Eq. (1))

$$\sum_{n=1}^{\infty} a_{2n} = 0 \,. \tag{3}$$

When limited to the first two leading terms, a_2 and a_4, the above equation allows, together with (2), to determine the scission line, then given by

$$a_4 + \frac{\pi}{4c} = 0 \,. \tag{4}$$

In the presence of odd-multipolarity deformations, one can make sure, through an adequate choice of the above introduced shift parameter $z_{\rm sh}$, that the centre of mass of the shape is always located at the origin of the coordinate system

$$z_{\rm cm} = \frac{\int_V z\, d^3r}{\int_V d^3r} = \frac{\pi \int_{z_{\rm min}}^{z_{\rm max}} \rho_{\rm s}^2(z)\, z\, dz}{\pi \int_{z_{\rm min}}^{z_{\rm max}} \rho_{\rm s}^2(z)\, dz} = 0 \tag{5}$$

which together with (1) leads to the following expression for the shift coordinate:

$$z_{\rm sh} = -\frac{z_0}{2} \frac{\sum_n (-1)^{n-1} \frac{a_{2n+1}}{n}}{\sum_n (-1)^{n-1} \frac{a_{2n}}{2n-1}} = \frac{3c^2}{2\pi} R_0 \sum_{n=1}^{\infty} (-1)^n \frac{a_{2n+1}}{n} \,, \tag{6}$$

where (2) has been used.

The relative distance between the mass centres of left (z_l) and right (z_r) fragments (see Fig. 1) is given by

$$R_{12} = \frac{\int_{z_{\rm neck}}^{z_{\rm max}} z\, d^3r}{\int_{z_{\rm neck}}^{z_{\rm max}} d^3r} - \frac{\int_{z_{\rm min}}^{z_{\rm neck}} z\, d^3r}{\int_{z_{\rm min}}^{z_{\rm neck}} d^3r} = \frac{\pi \int_{z_{\rm neck}}^{z_{\rm max}} \rho_{\rm s}^2(z)\, z\, dz}{\pi \int_{z_{\rm neck}}^{z_{\rm max}} \rho_{\rm s}^2(z)\, dz} - \frac{\pi \int_{z_{\rm min}}^{z_{\rm neck}} \rho_{\rm s}^2(z)\, z\, dz}{\pi \int_{z_{\rm min}}^{z_{\rm neck}} \rho_{\rm s}^2(z)\, dz}\,, \tag{7}$$

where $z_{\rm neck}$ determines the location of the plane which separates the two fragments. Considering first the case of symmetric fission, where all a_ν with odd ν vanish, and consequently $z_{\rm neck} = 0$, one obtains from Eq. (7)

$$R_{12} = 2\, R_0\, c \left[1 - \frac{6}{\pi^2}\, c \sum_{n=1}^{\infty} (-1)^{n-1} \frac{a_{2n}}{(2n-1)^2} \right] . \tag{8}$$

In the asymmetric case, we define the neck coordinate $z_{\rm neck}$ as the location, where the shape $\rho_{\rm s}^2(z)$, Eq. (1), has an extremum. Since such an extremum, in the case of a fissioning nucleus generally a minimum will always occur, even for reasonably strong asymmetry, close to the centre of the shape, we determine the coordinate $x_{\rm neck} = (z_{\rm neck} - z_{\rm sh})/z_0$ by a Taylor expansion of the sine and cosine functions around $x = 0$. From the condition $d\rho_{\rm s}^2(z)/dz = 0$, one then obtains the following expression for $x_{\rm neck}$

$$x_{\rm neck} = \frac{4}{\pi} \frac{\sum_n n\, a_{2n+1}}{\sum_n (2n-1)^2\, a_{2n}} \tag{9}$$

and $z_{\rm neck} = z_{\rm sh} + z_0\, x_{\rm neck}$. This procedure has been tested for a large variety of shapes and turns out to work very accurately as long as the shapes are not pathological, *i.e.* physically relevant in the fission process.

3. Potential energy surface of a charged liquid drop

In the liquid drop (LD) model, the deformation energy of a nucleus as function of its deformation is given by (see *e.g.* [6])

$$\frac{\Delta E({\rm def})}{E_{\rm surf}({\rm sph})} = B_{\rm surf}({\rm def}) - 1 + 2\chi [B_{\rm Coul}({\rm def}) - 1]\,, \tag{10}$$

where $\Delta E({\rm def}) = E_{\rm LD}({\rm def}) - E_{\rm LD}({\rm sph})$ is the difference between the energies of the deformed and the spherical nucleus, and χ is the fissility parameter defined as

$$\chi = \frac{E_{\rm Coul}({\rm sph})}{2 E_{\rm surf}({\rm sph})}\,, \tag{11}$$

where $E_{\rm surf}({\rm sph})$ and $E_{\rm Coul}({\rm sph})$ are respectively the surface and the Coulomb energies of the spherical nucleus. An example for such a LD deformation energy is presented for $\chi = 0.8$ in Fig. 2. One observes that the path to fission goes towards the lower right end of the (c, a_4) plane, where scission occurs. Such a presentation in a (a_2, a_4), or as shown here, in a (c, a_4) deformation space is not very convenient for practical calculations. We would, indeed, rather like to have the same interval of a_4 values for all values of c.

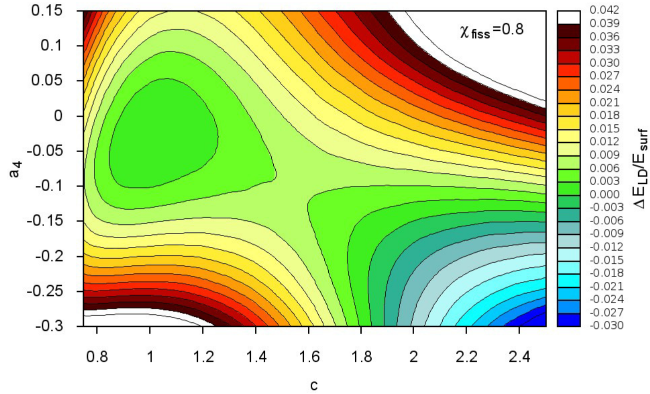

Fig. 2. Potential energy surface $\Delta E(\text{def})/E_{\text{surf}}(\text{sph})$ in the (c, a_4) plane for a nucleus with fissility parameter $\chi = 0.8$.

That is why we introduce new *rotated coordinates* (ξ, σ) in which the ξ-axis $(\sigma = 0)$ corresponds roughly to the fission path

$$\begin{cases} c - 1 &= \xi \cos \frac{\pi}{6} - \sigma \sin \frac{\pi}{6} \\ 3\, a_4 &= \xi \sin \frac{\pi}{6} + \sigma \cos \frac{\pi}{6} \end{cases} . \tag{12}$$

The potential energy surface, the same as in Fig. 2, but now in the new (ξ, σ) coordinate system is shown in Fig. 3.

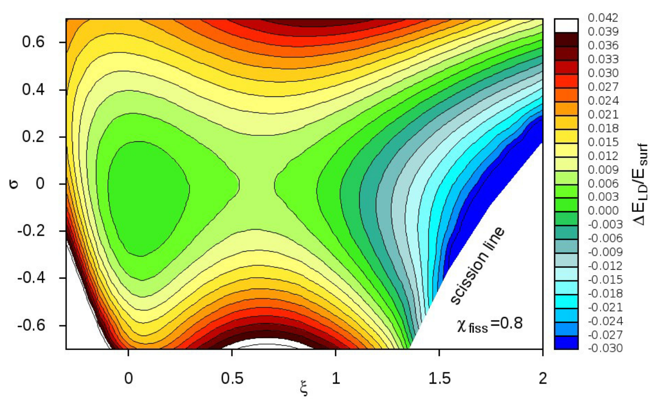

Fig. 3. The same as in Fig. 2 but on the (ξ, σ) plane.

The LD potential energy surface for reflection asymmetric shapes ($a_3 \neq 0$) is presented in Fig. 4 in the (ξ, a_3) plane. One concludes from this figure that a range of $-0.25 < a_3 < 0.25$ should be sufficient to describe the fission valley assuming the amplitude of the microscopic part of the energy in the asymmetry direction to be smaller than 5 MeV.

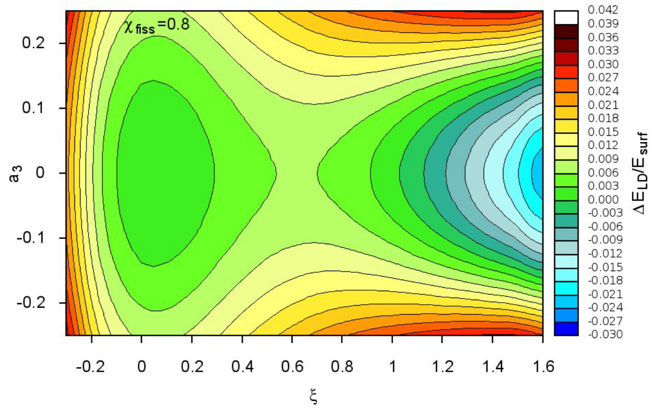

Fig. 4. The same as in Fig. 2 but on the (ξ, a_3) plane.

To evaluate the effect of higher order deformation term on the energy of the nucleus at the saddle and at the scission points, we have determined the LD energy in the (a_4, a_6) plane. The potential energy surfaces are shown in Figs. 5 and 6. One concludes from these results that taking the a_6 deformations into account decreases only slightly ($\sim$ 0.5 MeV) the energy of the saddle point (Fig. 5) and by about $\sim$1 MeV at the scission configuration (Fig. 6).

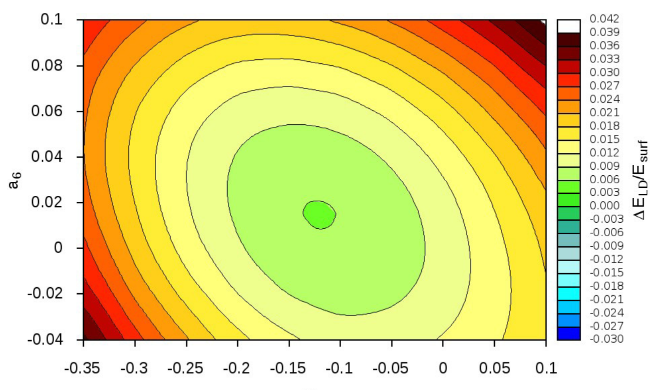

Fig. 5. LD potential energy surface on the (a_4, a_6) plane at the saddle point.

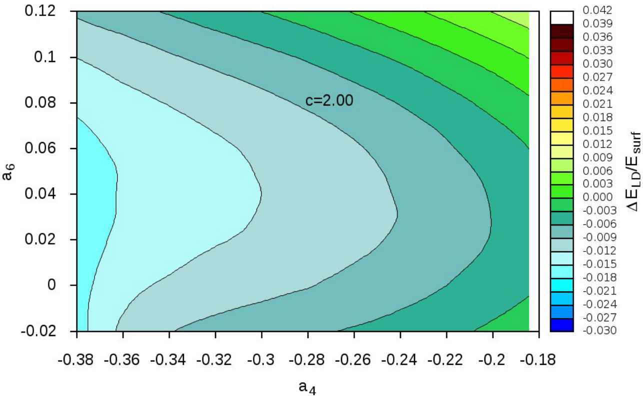

Fig. 6. The same as in Fig. 5 but around the scission configuration.

4. Summary

We have developed an efficient way to describe the shape of deformed nuclei using only a few deformation parameters. The new parametrization is equally efficient around the ground state as at very elongated nuclear shapes close to the scission configuration. The decomposition into the Fourier series of the square of the distance from the symmetry axis to the surface of the nucleus, not used before in the literature, is rapidly convergent. For many purposes, one can use only the first three deformation parameters: a_2 related to the elongation, a_3 responsible for the mass asymmetry and a_4 playing the role of the neck parameter. The higher deformation degrees of freedom can be easily added when a better precision of the calculations is desired. The new shape parametrization is especially suitable for the description of the fission process. The frequently used parametrization β_λ in spherical harmonics is not so rapidly converging, requiring the 7 first even β_λ parameters to obtain a proper description of the shape of the liquid drop fission barrier from the ground state until the scission point [2], while a similar accuracy is reached in the above presented Fourier decomposition taking into account only the three first even coefficients a_2, a_4, a_6.

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