TRANSPORT COEFFICIENTS WITHIN A FOURIER SHAPE PARAMETRIZATION*

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Dedicated to the memory of Adam Sobiczewski

Transport coefficients, such as the collective potential, inertia, friction and diffusion tensors, that are required in any dynamical description of the fission process are reviewed. These are mandatory when solving *e.g.* the Langevin equation that allows to follow the time evolution of a deformed, hot rotating nucleus from its formation in a heavy-ion collision up to the scission instability. The present study is carried out using a new shape parametrization which we have developed and which is based on a Fourier expansion of the nuclear shape function.

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1. Introduction

An accurate description of nuclear shapes relying only on very few collective parameters is a very challenging task, especially in connection with a large-amplitude collective motion, such as the fission process, which involves a huge variety of nuclear deformations, from ground-state shapes not far from sphericity up to very elongated and possibly necked-in configurations as they appear when reaching the scission instability. Many very powerful shape parametrizations have been developed in the past (see *e.g.* [1] for a review). Let us simply mention here the expansion in spherical harmonics due to Lord Rayleigh [2], still extremely popular nowadays in the nuclear physics community, but also the so-called *Funny Hills* parametrization [3] or the Trentalange–Koonin–Sierk shapes [4], which have both been very successful, in particular in connection with the fission process.

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We shall report here on the results of calculations concerning the transport coefficients which are the indispensable building blocks of the description of any dynamical process. The process which we have in particular in mind is the fission process, which we would like to depict by resolving the Langevin equation, *i.e.* a classical equation of motion, which contains, however, most of the quantum structure of the nuclear many-body problem, taking specially into account such complicated problems as the dissipation of collective energy into intrinsic (single-particle) excitation, as described by a friction term and the fluctuation of the collective coordinates, that appear in such a statistical approach through a diffusion term (see Ref. [5] for a review).

We are going to do that by using a parametrization of the nuclear deformation relying on a Fourier expansion of the nuclear shape, that we have recently developed [6, 7], and that has proven to be rapidly converging and to allow for a very accurate description of deformed nuclear shapes [8, 9]. We are thus able with only 4 collective variables that correspond to elongation, left–right asymmetry, non-axiality and neck formation to describe the above-mentioned very large variety of nuclear shapes that can possibly occur during the fission process. This shape parametrization has, *e.g.* allowed us in the past to account for the coexistence and the competition between different fission valleys generating different fission modes. We have thus been able to identify the coexistence of 3 different fission modes in heavy Fm isotopes, corresponding to a compact asymmetric, an elongated symmetric (so-called *superlong*) and a particularly compact symmetric mass split [7].

After introducing in some detail the above-mentioned Fourier shape parametrization in Section 2, we will give in Section 3 a brief description of the Langevin approach of dissipative dynamics and of the transport functions (also called coefficients) that enter the Langevin equation. In Section 4, we will explain how to determine these transport functions for any nuclear deformation and show some first results on their form and behaviour before concluding.

2. The Fourier shape parametrization

The capacity to define the deformation dependence of the energy of a nucleus in a simple yet efficient way, using as few collective coordinates as ever possible, is an extremely demanding task. What is, in addition, highly desirable is the capability to test its convergence. This is, *e.g.* the case of Lord Rayleigh's expansion of the nuclear radius $R(\theta, \varphi)$ in spherical harmonics [2], but not so for the famous *Funny Hills* (FH) shape parametrization [3] of the Copenhagen group, which is, however, much better suited to describe the shape of fissioning nuclei as demonstrated in Ref. [10]. Other shape parametrizations that have had a large success, in particular in relation with the fission process and that need to be quoted in this connection are the expansion in Legendre polynomials [4] of the square distance $\rho^2(z)$ of the nuclear surface from the symmetry z axis in cylindrical coordinates (exactly as for the FH shapes) of Trentalange, Koonin and Sierk, the quadratic surfaces of revolution of Nix [11] and the Cassini ovals of Pashkevich [12, 13], where the last two shapes have the disadvantage, just as the FH shapes, of not being *open*, *i.e.* not allowing to test their convergence. One fundamental advantage for the description of the fission process, as we see it, of *e.g.* the Funny Hills shapes over Lord Rayleigh's expansion in spherical harmonics is that it parametrizes the distance squared $\tilde{\rho}_{\mathrm{s}}^2(z)$ of a surface point to the symmetry z axis rather than the radius squared $R^2(\theta,\varphi)$ in spherical coordinates.

Having these two conditions in mind, *i.e.* to parametrize the square distance of a surface point to the symmetry axis and to allow for a test of convergence by increasing the number of parameters, we have found [6] that an expansion of $\tilde{\rho}_{\mathrm{s}}^2(z)$ in a Fourier series is

$$\frac{\tilde{\rho}_{\mathrm{s}}^2(u)}{R_0^2} = \sum_{n=1}^{\infty} \left[a_{2n} \cos\left(\frac{(2n-1)\pi}{2}\, u\right) + a_{2n+1} \sin\left(\frac{2n\pi}{2}\, u\right)\right] , \tag{2.1}$$

where R_0 is the radius of the corresponding spherical nucleus having the same volume and $u = (z - z_{\mathrm{sh}})/z_0$, where $2z_0$ is the length of the nucleus and z_{sh} a parameter that guarantees that the centre of mass of the shape is located at the origin of the coordinate system, yields an excellent description of nuclear shapes.

Non-axial shapes can be generated by assuming that the cross section of the nucleus perpendicular to the z axis has, at any z value, the form of an ellipsoid as shown in Fig. 1. It can be shown [14] that the profile function

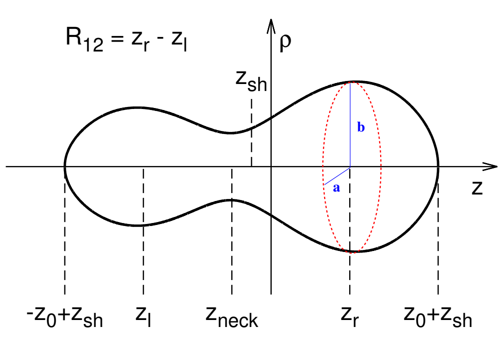

Fig. 1. Schematic visualization, in cylindrical coordinates, of the parameters entering the definition of the profile function defined by Eq. (2.2).

$\rho_s^2(z,\varphi)$ can then be written as

$$\rho_s^2(z,\varphi) \;=\; \tilde{\rho}_s^2(z)\; f(\varphi) \;=\; \tilde{\rho}_s^2[u(z)]\; \frac{1-\eta^2}{1+\eta^2+2\eta\cos(2\varphi)}\,, \tag{2.2}$$

where the non-axiality parameter η is a function of the coordinate z and defined by the ellipse half-axis $a(z)$ and $b(z)$ shown in the figure

$$\eta(z) = \frac{b(z)-a(z)}{b(z)+a(z)}\,, \qquad \text{where} \qquad a(z)\,b(z) \;=\; \rho_s^2(z)\;. \tag{2.3}$$

For the sake of simplicity, we will, however, assume in the following that η is a constant, *i.e.* is z-independent.

Considering the nucleus as an incompressible fluid, the condition that the volume of that body should stay constant in the deformation process allows to express the length $2z_0 = 2cR_0$ of the deformed nucleus through the relation

$$\sum_{n=1}^{\infty}(-1)^{n-1}\,\frac{a_{2n}}{2n-1} \;=\; \frac{\pi R_0}{3z_0}\,. \tag{2.4}$$

The condition that the centre of mass should be located at the origin of the coordinate system leads to the following expression for $z_{\rm sh}$:

$$z_{\rm sh} \;=\; \frac{3\,z_0^2}{2\pi R_0}\,\sum_{n=1}^{\infty}(-1)^n\,\frac{a_{2n+1}}{n}\,. \tag{2.5}$$

To illustrate the fast convergence of the Fourier expansion of deformed shapes, we show in Fig. 2 the contribution of different orders of that expansion for one left–right symmetric and one left– right asymmetric shape.

Even though this expansion is converging very rapidly, there are several minor details that can still be improved. As one can see from the table below, the lowest-order term for a spherical shape has a Fourier coefficient close to unity, while higher-order terms have very small, but non-vanishing contributions. These spherical Fourier coefficients are found to be given by

$$a_{2n}^{(0)} = (-1)^{n-1}\frac{32}{\pi^3\,(2n-1)^3} \qquad \text{and} \qquad a_{2n-1}^{(0)} = 0 \tag{2.6}$$

TABLE I

Values of the Fourier expansion coefficients $a_n^{(0)}$ for a spherical shape.

n	2	4	6	8	10
$a_n^{(0)}$	1.03205	−0.03822	0.00826	−0.00301	0.00142

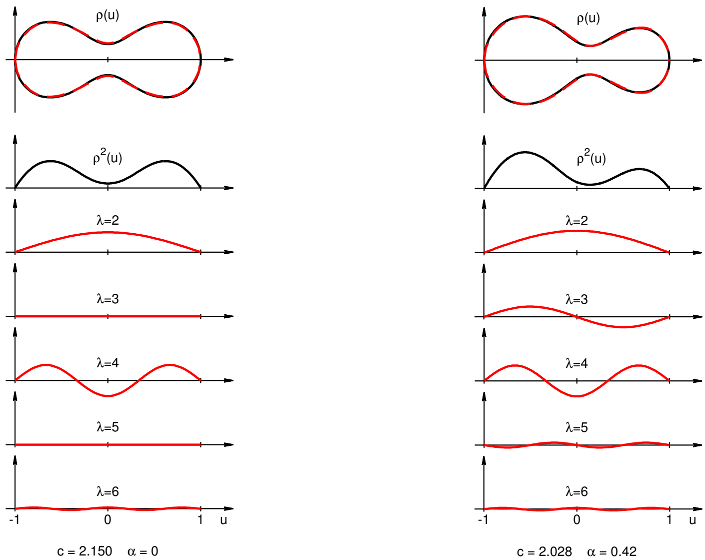

Fig. 2. Contribution of different orders of the Fourier expansion to the function $\rho_s^2(z)$ for a left–right symmetric (left) and one left–right asymmetric shape (right).

What is somehow unpleasant is that the quadrupole parameter a_2 decreases for increasing elongation, as can be seen from Eq. (2.4). To cure this little problem, one can introduce, as a function of the Fourier coefficients a_n, new deformation parameters q_n that all vanish for a spherical shape. This can, of course, be done in different ways. What we believe a clever way to proceed, is to define the new shape coefficients q_n in such a way that along the liquid-drop path to fission they all, except for the elongation parameter q_2, remain essentially zero. This leads to the following definition of the q_n:

$$q_2 = \frac{a_2^{(0)}}{a_2} - \frac{a_2}{a_2^{(0)}}\,, \qquad q_3 = a_3\,, \qquad q_4 = a_4 + \sqrt{\left(\frac{q_2}{9}\right)^2 + \left(a_4^{(0)}\right)^2}\,,$$

$$q_5 = a_5 - a_3\,\frac{q_2 - 2}{10}\,, \quad q_6 = a_6 - \sqrt{\left(\frac{q_2}{100}\right)^2 + \left(a_6^{(0)}\right)^2}\,. \tag{2.7}$$

It is clear that when taking quantum effects and pair correlations into account, higher order Fourier coefficients will not all stay exactly equal zero all along the path to fission, but take on some small, but non-vanishing values. We believe, however, that our way to introduce the new q_n collective coordinates is the best one can do to keep the number of these coordinates as small as ever possible and to be able to describe the entire path of the nuclear system from ground state to the scission instability with essentially three deformation parameters, one, q_2, for elongation, one left–right asymmetry parameter q_3 and one neck-formation parameter q_4 plus, if necessary, one non-axiality parameter η.

Using Eq. (2.2) and the above relations, all transport functions entering the Langevin equation can be evaluated as we will show in Section 4.

3. The Langevin equation of dissipative dynamics

Nuclear reactions such as the fusion or the fission process are very complex phenomena which are related to a large transfer of nuclear mass as well as a substantial transfer of nuclear energy from the collective to the single-particle degrees of freedom, which can be considered, in such an approach, as a heat reservoir. The derivative of the collective potential $V(\vec{q})$ with respect to the collective coordinate (here the deformation parameter) q_i plays the role of the driving force $F_i(\vec{q})$. The collective kinetic energy is a quadratic form of the collective velocities $\dot{q}_i$, the time derivatives of the collective coordinates describing the nuclear shape, with an inertia tensor $\mathcal{M}_{ij}$. The dissipation of collective energy into intrinsic (single-particle) excitation is described by the friction tensor γ_{ij}, and the fluctuations of the collective coordinates which appear in such a statistical approach by the diffusion tensor $\mathcal{D}_{ij}$.

In many applications, the dynamics of such a reaction is described by the Fokker–Planck equation [15] through the distribution probability $w(\vec{q},\vec{p},t)$ of finding a nucleus at a given point in the collective phase-space built from the deformation parameters q_i and conjugate momenta p_i

$$\begin{aligned}\frac{\partial w}{\partial t} &= \sum_i \frac{\partial V}{\partial q_i}\frac{\partial w}{\partial p_i} - \sum_{i,j} \mathcal{M}^{-1}_{ij}\, p_i \,\frac{\partial w}{\partial q_j} \\ &\quad + \sum_{i,j}\frac{\partial}{\partial p_i}\left[\sum_k \gamma_{ik}\,\mathcal{M}^{-1}_{kj}\, p_j\, w\right] + \sum_{i,j}\mathcal{D}_{ij}\,\frac{\partial^2 w}{\partial p_i\,\partial p_j}\,. \end{aligned} \tag{3.1}$$

It has been shown (see, *e.g.* [15]) that such a transport equation, derived on the basis of statistical (stochastic) mechanics, is equivalent to a Langevin equation with a normally distributed random force

$$\begin{aligned}\frac{\mathrm{d}q_i}{\mathrm{d}t} &= \sum_j \mathcal{M}^{-1}_{i,j}\, p_j\,, \\ \frac{\mathrm{d}p_i}{\mathrm{d}t} &= -\,\frac{\mathrm{d}V}{\mathrm{d}q_i} - \frac{1}{2}\sum_{j,k}\frac{\mathrm{d}\mathcal{M}^{-1}_{jk}}{\mathrm{d}q_i}\, p_j\, p_k - \sum_{j,k}\gamma_{ij}\,\mathcal{M}^{-1}_{jk}\, p_k + \mathcal{F}^{\mathrm{L}}_i(\vec{q},t)\,,\end{aligned} \tag{3.2}$$

where $\mathcal{F}_i^{\mathrm{L}}$ is the Langevin random force defined as

$$\mathcal{F}_i^{\mathrm{L}}(\vec{q},t) = \sum_j g_{ij}(\vec{q})\, \mathit{\Gamma}_j(t)\,, \tag{3.3}$$

with the diffusion tensor

$$\mathcal{D}_{ij} = \sum_k g_{ik}\, g_{kj} \tag{3.4}$$

and Gaussian-distributed random numbers $\mathit{\Gamma}_j(t)$ with vanishing mean value $\langle \mathit{\Gamma}_j(t) \rangle$ and delta-correlated variance

$$\left\langle \mathit{\Gamma}_i(t)\, \mathit{\Gamma}_j\left(t'\right) \right\rangle = 2\, \delta_{ij}\, \delta\left(t - t'\right)\,. \tag{3.5}$$

One can then determine the transport coefficients $V(\vec{q})$, $\mathcal{M}_{ij}$, γ_{ij} and $\mathcal{D}_{ij}$ that enter the Langevin equation governing the time evolution of the nuclear system. This is what is going to be done now.

4. The transport functions of the Langevin equation

As immediately seen from Eq. (3.2), the Langevin equation that we plan to solve, is a classical Hamilton-type equation of motion for the collective coordinates q_i and the associated conjugate momenta p_i. It is clear that in a multidimensional coordinate space, quantities such as the collective mass and the friction coefficient are going to be tensors rather than simple coefficients, just as the driving force is going to be determined by the components of the gradient of the collective potential describing the deformation energy of our nuclear system. The first and probably the most important quantity that needs to be determined is, therefore, this collective potential $V(\vec{q})$, which is calculated as the nuclear deformation energy, *i.e.* the energy of the deformed nucleus relative to the energy at the spherical configuration

$$V(\vec{q}, T, L) = F(\vec{q},\, T, L) - F(\vec{q} = 0, T = 0, L = 0)\,. \tag{4.1}$$

Notice, please, that instead of the total energy E of the nuclear system, we have written here the Helmholtz free energy F given by

$$F(\vec{q},\, T, L) \;=\; E(\vec{q},\, L) - a(\vec{q})\, T \tag{4.2}$$

with $a(\vec{q})$ the deformation-dependent level-density parameter (see, *e.g.* [10]).

Since, as already mentioned in the preceding section, fusion as well as the fission process involve the transfer of particles, but also of energy between the collective and the intrinsic degrees of freedom, it turns, indeed, out indispensable to take the nuclear excitation into account. This is done here by a description of the excited nuclear system as part of a grand-canonical ensemble. One has, however, to keep in mind that excitation cannot only be of thermal, but also of rotational origin, since the compound nuclear system that one is studying has, *e.g.* been formed in a heavy-ion collision with non-zero impact parameter and might, therefore, carry a non-negligible amount of rotational angular momentum L, what we have taken into account in Eqs. (4.1) and (4.2).

To calculate the nuclear energy, we rely on the macroscopic–microscopic approach

$$E_{\rm mac}(\vec{q},\,L) = E_{\rm mac}(\vec{q},\,L) + E_{\rm mic}(\vec{q},\,L)\,, \tag{4.3}$$

where the Lublin–Strasbourg Drop model [16] is used for the liquid-drop-type energy, including a curvature $A^{1/3}$ term in the leptodermous expansion and a deformation-dependent congruence energy term [17, 18]. This approach has been demonstrated [16] to yield precise nuclear ground-state masses and fission-barrier heights

$$E_{\rm mac}(\vec{q},\,L) = E_{\rm vol} + E_{\rm surf}(\vec{q}) + E_{\rm cur}(\vec{q}) + E_{\rm Coul}(\vec{q}) + E_{\rm cngr}(\vec{q}) + E_{\rm rot}(\vec{q},L)\,, \tag{4.4}$$

where the deformation dependence of the different terms is calculated [1] through shape functions B_i that express the corresponding energy contribution E_i relative to the one at the spherical shape, like $E_{\rm surf}(\vec{q}) = B_{\rm surf}(\vec{q}) E_{\rm surf}(\vec{q}=0)$. These shape functions B_i are entirely determined by the density profile functions $\rho_{\rm s}^2(z,\varphi)$ of Eq. (2.2). The nucleus being considered as an essentially incompressible fluid, the volume term is, of course, deformation-independent.

The microscopic part in (4.3) is obtained with the Strutinsky shell-correction method [19] using single-particle levels of a Yukawa-folded mean field and the BCS theory with a constant pairing strength seniority force [20] to account for the pairing correlations.

As an illustration, we show in Fig. 3, the deformation energy of the nucleus ^{228}Ra in the (q_2, q_3) plane. One clearly identifies the nuclear ground state at a prolate deformation of $q_2 \approx 0.35 > 0$ which is left–right symmetric $(q_3 = 0)$, a fission isomeric state at $q_2 \approx 0.80$, again left–right symmetric, a second barrier which is higher that the first, but which is obviously overcome by going through left–right asymmetric shapes before reaching the scission configuration somewhere beyond $q_2 \approx 2.1$. One obviously observes here two fission valleys, one symmetric and the other asymmetric where the asymmetric valley seems to be deeper than the symmetric one. We thus expect some bimodal fission in ^{236}Pu with an asymmetric fission that dominates. Let us mention here that this deformation energy landscape has been given just as an example about what information can be obtained when looking at such deformation energies. Even though the landscape shown here has been obtained for a nucleus at zero temperature and zero angular momentum, we need to insist here on the fact that similar results can, of course, be obtained for nuclear systems with thermal or rotational excitation (or both).

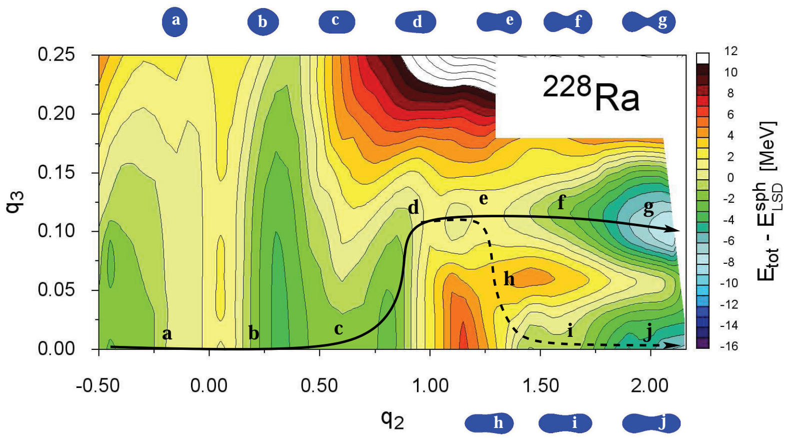

Fig. 3. Deformation energy landscape of the nucleus ^{228}Ra as a function of the elongation q_2 and left–right asymmetry coordinate q_3. In all the deformation points of this plane, the energy has been minimized with respect to the neck parameter q_4. Some selected shapes are displayed on top and bottom of the landscape.

Let us now turn to the other ingredients of the Langevin or Fokker–Planck equation, namely the collective mass, the friction and the diffusion tensor. In the approach of an irrotational flow, the inertia tensor is expressed in the Werner–Wheeler approximation [21] as

$$\mathcal{M}_{ij} = \rho_0 \int\limits_V \left[\left(A_i^\rho\, A_j^\rho + A_i^\varphi\, A_j^\varphi \right) \rho_\mathrm{s}^2(z,\varphi) + A_i^z\, A_j^z \right] \mathrm{d}^3 r\,, \qquad (4.5)$$

where the A_j^ν are the expansion coefficients of the velocity field in ν direction ($\nu = z, \rho, \varphi$) which are derived in Ref. [22].

At not too small temperatures, the friction tensor is well-approximated by the wall formula [23]

$$\gamma_{ij} = \frac{\rho_0}{2}\, \bar{v} \int\limits_{z_\mathrm{min}}^{z_\mathrm{max}} \mathrm{d}z \int\limits_0^{2\pi} \mathrm{d}\varphi\, \frac{\frac{\partial \rho_\mathrm{s}^2}{\partial q_i}\, \frac{\partial \rho_\mathrm{s}^2}{\partial q_j}}{\sqrt{4\rho_\mathrm{s}^2 + \frac{1}{\rho_\mathrm{s}^2}\left(\frac{\partial \rho_\mathrm{s}^2}{\partial \varphi}\right)^2 + \left(\frac{\partial \rho_\mathrm{s}^2}{\partial z}\right)^2}} \qquad (4.6)$$

frequently used in dissipative-dynamics calculations related to the fission of thermally excited nuclei, where ρ_0 is a uniform density and $\bar{v}$ some average nucleon velocity.

The diffusion tensor is finally obtained in our approach through the Einstein relation

$$\mathcal{D}_{ij} = T\,\gamma_{ij}\,, \tag{4.7}$$

a relation that should be a good approximation at high nuclear temperatures T.

The mass, friction and diffusion tensors derived in this way have been obtained in the space of the Fourier parameters a_k. What we are finally interested in, however, are the expressions of these quantities as expressed in the space of our new collective coordinates q_ν, since it is in that space that we are going to solve the Langevin equation. The transformation from the a_k space to the q_ν space is given by the following equations:

$$\mathcal{M}_{\mu\nu} = \sum_{k,\ell} \mathcal{M}_{k\ell}\,\frac{\partial a_k}{\partial q_\mu}\,\frac{\partial a_\ell}{\partial q_\nu} \qquad \text{and} \qquad \gamma_{\mu\nu} = \sum_{k,\ell} \gamma_{k\ell}\,\frac{\partial a_k}{\partial q_\mu}\,\frac{\partial a_\ell}{\partial q_\nu}\,. \tag{4.8}$$

Let us show in the following some of the components of the resulting mass and friction tensors. These components are universal in the sense that they do not depend on the specific nucleus studied, except for a trivial dependence

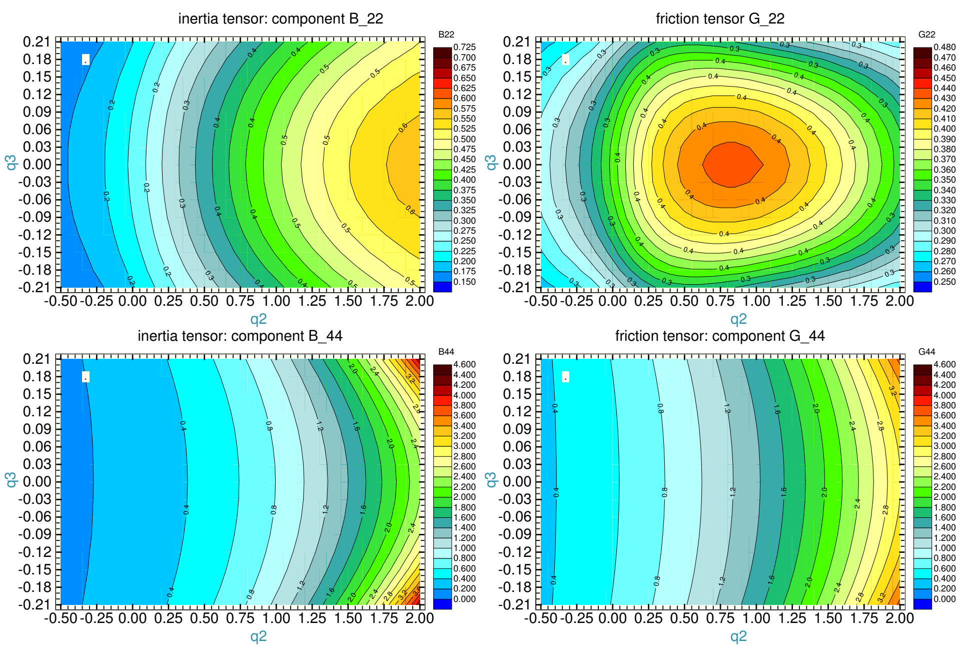

Fig. 4. Components of the inertia (left) and the friction tensor (right column) in the (q_2, q_3) plane corresponding respectively to the elongation and left–right asymmetry degree of freedom. The diagonal components for elongation (top) and neck degree of freedom (bottom row) are shown.

on the nucleon number A, but only of the shape profile functions $\rho_{\rm s}^2(z,\varphi)$. We thus show in Fig. 4 the diagonal components B_{22} and B_{44} of the mass tensor corresponding to the elongation and the neck degree of freedom, as well as for the corresponding components G_{22} and G_{44} of the friction tensor.

5. Conclusions

A new very rapidly converging Fourier expansion that allows for a very versatile description of nuclear shapes, in particular for the large variety of nuclear deformations encountered in the fission process, is used to produce deformation energy surfaces that are able to describe such fine details as the coexistence of different fission valleys leading to different fission channels. In addition, we have presented the expressions for the components of inertia, friction and diffusion tensors corresponding to the degrees of freedom defined by this shape parametrization and that correspond to elongation, left–right asymmetry, neck formation and non-axiality. The next step should now be to incorporate all these transport functions into the Langevin equation to allow for the description of the dynamics of the fission process. This Langevin equation will be coupled to Master equations to account for the possible de-excitation of the compound nucleus through the evaporation of particles (n,p,α), but also of γ rays. Such a de-excitation process leads to a cooling of the system which can thus end up as a *evaporation residue*, a process which could be of great importance for the synthesis of super-heavy elements. Work along this direction is under way.

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