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# Transport coefficients in the Fourier shape parametrization ☆

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ABSTRACT

An innovative parametrization of nuclear shapes, based on a Fourier expansion of the square distance from the surface of the nucleus to the symmetry axis is introduced. Surface, curvature and Coulomb energy coefficients of a charged liquid drop, that determine the semiclassical nuclear energy, are evaluated within this shape parametrization, together with the wall-friction and the irrotational-flow mass tensors. These transport coefficients are important ingredients of many nuclear models describing nuclear structure and dynamics. A numerical code allowing for the determination of all these quantities for a huge variety of nuclear shapes is made available to the interested user.

**Program summary**

*Program title:* inerfric
*Program Files doi:* http://dx.doi.org/10.17632/gtvbc8b7sw.1
*Licensing provisions:* GPLv3
*Programming language:* Fortran
*Nature of problem:* The inertia tensor evaluated in the hydrodynamical model using the Werner–Wheeler approximation generalized to nonaxial shapes is evaluated, together with the friction tensor using the wall formula, and the shape functions that define the liquid-drop energy in terms of surface, curvature, Coulomb and congruence energy. For the description of the fission process, the mass ratio of the nascent fission fragments and their centre-of-mass distance is also evaluated together with the quadrupole moment and the moments of inertia for rotation of the deformed shape.
*Solution method:* All these quantities are evaluated in our new rapidly converging Fourier shape parametrization, able to describe a huge variety of nuclear shapes, simply by reading in the (up to 7) shape parameters determining in an unambiguous way the nuclear deformation and corresponding for the (4) principal parameters to the nuclear elongation, left–right asymmetry, non axiality and neck degree of freedom, the remaining 3 allowing, if necessary, to optimize the evaluation of the asymmetry and neck degrees of freedom.



## 1. Introduction

An accurate description of nuclear shapes which involves as few collective variables as ever possible is a very demanding task, especially in connection with the fission process, which involves an impressive variety of nuclear shapes. Several powerful shape parametrizations have been developed in the past [1]. We will use here a recently developed parametrization which allows to cover a rich variety of shapes with four collective deformation parameters only [2]. This parametrization based on a Fourier expansion of the square distance of any point on the nuclear surface to the symmetry axis (chosen here as the $z$-axis) is very rapidly converging and easy to handle. In addition, it is able to overcome some of the limitations encountered with previous prescriptions. A detailed analysis of the deformation-energy landscapes, limited to only 4 deformation parameters is thus presented in this work.

The investigations carried out in Refs. [2,3] demonstrate the high performance of the here proposed approach and enables us to study large amplitude collective phenomena in a rather accurate way, often better as compared to those carried out with more *advanced* models involving a much larger number of deformation parameters, which, to our understanding, seems to indicate that our approach contains the *essential* physical ingredients. Our approach can be implemented very easily into any extended dynamical calculations of nuclear potential-energy surfaces as well as into the dynamical calculation related to the nuclear fission or fusion process. In particular, one could have in mind the Langevin

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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approach of dissipative dynamics, coupled with the evaporation of light particles (see e.g. [4–6] and references therein).

Section 2 presents a brief summary of the Langevin approach of dissipative dynamics and of all transport functions (frequently called coefficients) entering the Langevin equation. In Section 3 we give detailed expressions for the liquid-drop shape-dependent coefficients and some global macroscopic quantities characterizing the nuclear mater distribution, like the density multipole moments and the moments of inertia. Section 4 gives the expressions of the nuclear friction tensor and the irrotational-flow mass tensor in our Fourier shape parametrization. At the end we present in Section 5 the description of the computer code that allows to evaluate the above transport coefficients and we give a few typical examples with their results. A detailed derivation of the velocity field of an irrotational flow is described in the Appendix.

## 2. Langevin dissipative dynamics

Nuclear reactions like 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 built from the inertia tensor $\mathcal{M}_{ij}$ and the collective velocities $(\dot{q}_i)$ which are the time derivatives of the collective coordinates describing the nuclear shape. The dissipation of collective energy into intrinsic (single-particle) excitation is described by the friction tensor $\gamma_{ij}$, and the fluctuations of the collective coordinates which appear in such a statistical approach by the diffusion tensor $\mathcal{D}_{ij}$.

In many applications, it is assumed that 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 $p_i$ is described by the Fokker–Planck equation [7]:

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

It has been shown (see e.g. [7]) 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. One can then determine the transport coefficients that enter the Langevin equation governing the time evolution of the nuclear system

$$\begin{cases} \dfrac{dq_i}{dt} = \displaystyle\sum_j \mathcal{M}^{-1}_{i,j}\, p_j \quad , \\ \dfrac{dp_i}{dt} = -\dfrac{dV}{dq_i} - \dfrac{1}{2}\displaystyle\sum_{j,k} \dfrac{d\mathcal{M}^{-1}_{jk}}{dq_i}\, p_j\, p_k \\ \qquad\quad - \displaystyle\sum_{j,k} \gamma_{ij}\, \mathcal{M}^{-1}_{jk}\, p_k + \mathcal{F}^{(L)}_i(\vec{q}, t) \quad . \end{cases} \tag{2}$$

Here $\mathcal{F}^{(L)}_i$ is the Langevin random force defined as

$$\mathcal{F}^{(L)}_i(\vec{q}, t) = \sum_j g_{ij}(\vec{q}\,)\, \Gamma_j(t)\,, \tag{3}$$

where

$$\sum_k g_{ik}\, g_{kj} = \mathcal{D}_{ij} \tag{4}$$

and $\Gamma_j(t)$ are Gaussian-distributed random numbers with vanishing mean value $\langle \Gamma_j(t) \rangle$ and delta-correlated variance

$$\langle \Gamma_i(t)\, \Gamma_j(t') \rangle = 2\, \delta_{ij}\, \delta(t - t')\,. \tag{5}$$

In the following section we are going to collect the expressions that allow to evaluate, in a macroscopic approximation, all the transport functions entering the Fokker–Planck (1) or Langevin (2) equations.

## 3. The transport function in the Fourier shape parametrization

The deformation dependent transport functions, like the nuclear collective potential-energy surface, collective inertia, friction and diffusion tensors, which enter the Langevin or Fokker–Planck equations should be evaluated using a given shape parametrization. In our present study we use the Fourier parametrization of deformed shapes written in cylindrical coordinates $(\rho, \varphi, z)$, a parametrization that is not only rapidly converging as was shown in Ref. [2], but it is also simple, analytical and *not closed*, which means that its convergence can be tested (contrary e.g. to the famous *Funny-Hills* shape parametrization [8]). To our opinion this is one of the best parametrizations which can be used both in nuclear-structure and nuclear-dynamics calculations.

The surface of an axially symmetric nucleus, or more precisely the square distance of a surface point to the symmetry $z$-axis, can be expanded in a Fourier series in the following way [2]:

$$\frac{\tilde{\rho}^2_s(u)}{R_0^2} = \sum_{n=1}^{\infty}\left[a_{2n}\cos\left(\frac{(2n-1)\pi}{2}\,u\right) + a_{2n+1}\sin\left(\frac{2n\pi}{2}\,u\right)\right] \tag{6}$$

where $R_0$ is the radius of a spherical nucleus having the same volume as the deformed one and $u = (z - z_{sh})/z_0$, where $2z_0$ is the length of the nucleus and $z_{sh}$ is a parameter that guarantees that the nuclear centre of mass is located at the origin of the coordinate system.

More general nonaxial shapes can be obtained by assuming that any cross-section of the nucleus perpendicular to the $z$-axis has the form of an ellipsoid as shown in Fig. 1:

$$\rho^2_s(z,\varphi) \;=\; \tilde{\rho}^2_s(z) f(\varphi) \;=\; \tilde{\rho}^2_s[u(z)]\,\frac{1-\eta^2}{1+\eta^2+2\eta\cos(2\varphi)}\,. \tag{7}$$

Here the non-axiality parameter $\eta$ is a function of the coordinate $z$ and defined by the ellipse half-axis $a(z)$ and $b(z)$:

$$\eta(z) = \frac{b(z)-a(z)}{b(z)+a(z)} \qquad \text{where} \qquad a(z)\cdot b(z) \;=\; \rho^2_s(z)\,. \tag{8}$$

For the sake of simplicity, we will assume in the following that $\eta$ is a constant.

The nucleus being considered as an essentially incompressible fluid, the volume-conservation condition requires that

$$\int_{-z_0+z_{sh}}^{z_0+z_{sh}} dz \int_0^{2\pi} d\varphi \int_0^{\rho(z)} \rho\, d\rho \;=\; \frac{4\pi}{3}R_0^3\,, \tag{9}$$

what leads to the relation:

$$\sum_{n=1}^{\infty}(-1)^{n-1}\,\frac{a_{2n}}{2n-1} \;=\; \frac{\pi R_0}{3z_0}\,. \tag{10}$$

The above equation allows to evaluate the length of the deformed nucleus. The condition that the centre of mass should be located at the origin of the coordinate system leads to the following expression for $z_{sh}$:

$$z_{sh} \;=\; \frac{3\,z_0^2}{2\pi R_0}\sum_{n=1}^{\infty}(-1)^n\,\frac{a_{2n+1}}{n}\,. \tag{11}$$

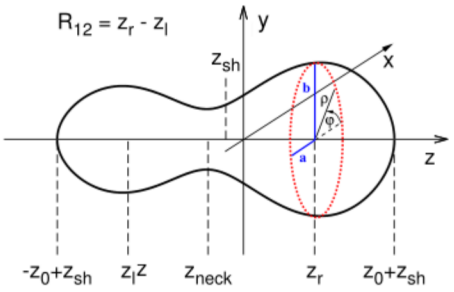


**Fig. 1.** (Colour online) Schematic visualization, in cylindrical coordinates, of the parameters entering the definition of the profile function defined by Eq. (7).

Using Eq. (7) and the above relations one can evaluate all transport functions entering the Langevin or Fokker–Planck equations.

One usually assumes that the Einstein relation

$$\mathcal{D}_{ij} \;=\; \gamma_{ij}\, T \;\;, \tag{12}$$

between the diffusion and the friction tensor holds, where $T$ is the nuclear temperature. At larger temperatures the friction tensor is well approximated by the wall-formula [9]

$$\gamma_{ij} = \frac{\rho_0}{2}\,\bar{v}\int_{z_{\min}}^{z_{\max}} dz \int_0^{2\pi} d\varphi\, \frac{\frac{\partial\rho_s^2}{\partial q_i}\,\frac{\partial\rho_s^2}{\partial q_j}}{\sqrt{4\rho_s^2+\frac{1}{\rho_s^2}\left(\frac{\partial\rho_s^2}{\partial\varphi}\right)^2+\left(\frac{\partial\rho_s^2}{\partial z}\right)^2}} \tag{13}$$

frequently used in dissipative-dynamics calculations related to the fission of hot nuclei. The irrotational flow inertia-tensor in the Werner–Wheeler approximation [10] can be written as

$$\mathcal{M}_{ij} = \rho_0 \int_V \left[\left(A_i^\rho\, A_j^\rho + A_i^\varphi\, A_j^\varphi\right)\rho_s^2(z,\varphi) + A_i^z\, A_j^z\right] d^3r \;, \tag{14}$$

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

The potential energy of a deformed (deformation parameters $\vec{q}$), hot (temperature $T$) and rotating (angular momentum $L$) nucleus is defined by the difference of the Helmholtz free energies $F$ between deformed and spherical nucleus:

$$V(\vec{q}\,,T,L) = F(\vec{q},\;T,L) - F(\vec{q}=0,T,L) \tag{15}$$

where the free energy is given by

$$F(\vec{q},\;T,L) \;=\; E(\vec{q},\;L) - a(\vec{q}\,)T \tag{16}$$

with $a(\vec{q}\,)$ the deformation dependent level-density parameter (see e.g. [11]).

In the approximation where the nucleus can be considered as a charged liquid drop, the nuclear energy is given as the sum of volume, surface, curvature, Coulomb, and rotational energies:

$$E(\vec{q},\;L) = E_{\rm vol} + E_{\rm surf}(\vec{q}\,) + E_{\rm cur}(\vec{q}\,) + E_{\rm Coul}(\vec{q}\,) + E_{\rm rot}(\vec{q}\,,L)\;, \tag{17}$$

The first term, the volume term, in Eq. (17) is deformation independent (the nucleus is considered to be incompressible), while the variation with deformation of all the other energy contributions can be described by the following dimensionless functions:

$$\begin{aligned} B_{\rm surf}(\vec{q}\,) &= E_{\rm surf}(\vec{q}\,)/E_{\rm surf}({\rm sph})\;,\\ B_{\rm cur}(\vec{q}\,) &= E_{\rm cur}(\vec{q}\,)/E_{\rm cur}({\rm sph})\;,\\ B_{\rm Coul}(\vec{q}\,) &= E_{\rm Coul}(\vec{q}\,)/E_{\rm Coul}({\rm sph})\;. \end{aligned} \tag{18}$$

Taking derivatives of the profile function (7), one is able to determine the shape functions corresponding to the surface energy

$$B_{\rm surf} = \frac{1}{4\pi R_0^2}\int_{-z_0}^{z_0} dz \int_0^{2\pi} d\varphi\, \sqrt{\rho_s^2(z,\varphi)+\left(\frac{\partial\rho_s}{\partial\varphi}\right)^2+\left(\rho_s\,\frac{\partial\rho_s}{\partial z}\right)^2}\;, \tag{19}$$

to the curvature energy

$$\begin{aligned} B_{cur} \;&= \frac{1}{8\pi R_0}\int_{z_{\min}}^{z_{\max}} dz \int_0^{2\pi} d\varphi \left[\rho_s^2+\rho_s^2\left(\frac{\partial\rho_s}{\partial z}\right)^2+\left(\frac{\partial\rho_s}{\partial\varphi}\right)^2\right]^{-1}\\ &\cdot\left\{\rho_s^2\left(\frac{\partial\rho_s}{\partial z}\right)^2-\rho_s\left(\frac{\partial\rho_s}{\partial z}\right)^2\frac{\partial^2\rho_s}{\partial\varphi^2}+\rho_s^2-\rho_s\frac{\partial^2\rho_s}{\partial\varphi^2}+2\left(\frac{\partial\rho_s}{\partial\varphi}\right)^2\right.\\ &\left.+2\,\frac{\partial\rho_s}{\partial z}\,\frac{\partial\rho_s}{\partial\varphi}\,\rho_s\,\frac{\partial^2\rho_s}{\partial z\partial\varphi}-\rho_s^3\,\frac{\partial^2\rho_s}{\partial z^2}-\rho_s\,\frac{\partial^2\rho_s}{\partial z^2}\left(\frac{\partial\rho_s}{\partial\varphi}\right)^2\right\}\;, \end{aligned} \tag{20}$$

and to the Coulomb energy

$$\begin{aligned} B_{\,Coul} &= \frac{5}{64\,\pi^2\,R_0^5}\int_{z_{\min}}^{z_{\max}} dz \int_0^{2\pi} d\varphi \int_{z_{\min}}^{z_{\max}} dz' \int_0^{2\pi} d\varphi'\\ &\cdot\left[\rho_s^2+\rho_{s'}^2-2\,\rho_s\,\rho_{s'}\cos(\varphi-\varphi')+(z-z')^2\right]^{-1/2}\\ &\cdot\left(\rho_s^2-\rho_s\rho_{s'}\cos(\varphi-\varphi')-\rho_{s'}\sin(\varphi-\varphi')\frac{\partial\rho_s}{\partial\varphi}-\rho_s(z-z')\,\frac{\partial\rho_s}{\partial z}\right)\\ &\cdot\left(\rho_{s'}^2-\rho_{s'}\rho_s\cos(\varphi-\varphi')+\rho_s\,\sin(\varphi-\varphi')\frac{\partial\rho_{s'}}{\partial\varphi'}+\rho_{s'}\,(z-z')\,\frac{\partial\rho_{s'}}{\partial z'}\right), \end{aligned} \tag{21}$$

where $\rho_{s'}$ is to be understood as a function of $z'$ and $\varphi'$.

One finally needs to take the rotational degree of freedom into account. In our semiclassical approach, the rotational energy is given by

$$E_{\rm rot}(\vec{q}\,) = \frac{L^2}{2\mathcal{J}(\vec{q}\,)}\;, \tag{22}$$

where $L$ is the angular momentum and $\mathcal{J}$ the moment of inertia with respect to the rotation axis. The relative change of the rotational energy with deformation is then simply

$$B_{\rm rot} = \frac{E_{rot}(\vec{q}\,)}{E_{rot}({\rm sph})} = \frac{\mathcal{J}({\rm sph})}{\mathcal{J}(\vec{q}\,)}\;, \tag{23}$$

where $\mathcal{J}$(sph) is the moment of inertia of the spherical nucleus. For a rotation around the $x$-axis, the parameter $B_{\rm rot}$ is given, in the rigid-body approximation, by the following expression:

$$B_{\rm rot} = \frac{32\,\pi\,R_0^5}{15}\left[\int_{z_{\min}}^{z_{\max}} dz \int_0^{2\pi} d\varphi\;[\,2\,z^2\tilde{\rho}_s^2+\tilde{\rho}_s^4\;\sin^2(\varphi)\,]\;\right]^{-1}. \tag{24}$$

All above functions entering the Langevin equation (2) and the macroscopic part of the collective potential (15) can be evaluated using the numerical program described in the next section which extensively uses the Fourier parametrization (7) of nuclear shapes.

## 4. Description of the numerical program

The computer code **inerfric.f** attached to the present paper is written according to the FORTRAN 90 and FORTRAN 95 standards. The module "*constants*" contains all physical and mathematical parameters used in the computer code. The parameters 'ng1', 'ng2', 'ng3' denote the order of the Gauss–Legendre integration quadratures (with ng1 $\neq$ ng3 to avoid divergencies in the calculation of the Coulomb energy), while 'no' gives the number of mesh points used in the rectangular (Romberg) integrations. All these parameters can, of course, be freely adjusted by the user. The values proposed in the code have, however, been tested and turned out to be sufficient to obtain the numerical results with the chosen accuracy (we have e.g. required the LDM energies to be determined with an accuracy better than 0.1 MeV). If desired

by the user, he can easily chose to improve that accuracy. The dimensionality 'ndim' of the $\{q_i\}$ deformation space is originally set to 'ndim = 6', but can be extended by the user up to 'ndim = 9'. Single-precision words are used in the program, but it is strongly recommended to compile it with the autodouble option in order to obtain the necessary precision of the transport coefficients needed in nuclear-physics calculations. Within the Linux system that would be:

*gfortran -fdefault-real-8 -o inerfric inerfric.f*

The command

*./inerfric < inerfric.inp > inerfric.out&*

would then execute the program taking the input data from the **inerfric.inp** file and storing the results into the **inerfric.out** file.

The code allows to evaluate the deformations dependent liquid-drop surface (BS), (first order) curvature (BK), Coulomb (BC) and rotational energy coefficients (Bx,Bz) for rotation around the $x$- and $z$-axes, respectively. In addition it gives the deformation dependence of the Wigner (congruence) energy (BW) according to Ref. [12], fission fragment mass ratio (BF) as well as the relative distance (R12) between the fragments, the length of nucleus (c) and the neck radius (Rn) in units of the spherical radius ($R_0$) and the quadrupole moment of the nucleus in $R_0^2$ units times the total mass or total charge of the nucleus. All above deformation dependent functions are evaluated in the subroutine "*fcs*".

The inertia tensor in the irrotational flow approximation and the wall friction tensor are evaluated as well in the subroutine "*tcoef* ". These tensors $T_{ij}$ being symmetric, only the upper part ($j \geq i$) needs to be evaluated in the four dimensional deformation-parameter space composed of non-axiality ($q_1 = \eta$), elongation ($q_2$), left–right asymmetry ($q_3$) and neck ($q_4$) degrees of freedom. One defines new collective coordinates

$$\begin{aligned} q_2 &= a_2^{(0)}/a_2 - a_2/a_2^{(0)} , & q_3 &= a_3 , \\ q_4 &= a_4 + \sqrt{((q_2/9)^2 + (a_4^{(0)})^2)} , & q_5 &= a_5 - (q_2 - 2)a_3/10 , \\ q_6 &= a_6 - \sqrt{((q_2/100)^2 + (a_6^{(0)})^2)} , & q_8 &= a_8 + \sqrt{((q_2/300)^2 + (a_8^{(0)})^2)} , \end{aligned} \tag{25}$$

where the

$$a_{2n}^{(0)} = (-1)^{n-1} \frac{32}{\pi^3 (2n-1)^3} \qquad \text{and} \qquad a_{2n-1}^{(0)} = 0 \tag{26}$$

are the Fourier components of the spherical shape.

The new parameters $q_i$ are chosen in such a way that the situations where all $q_i$ vanish correspond to the spherical shape of the nucleus. Oblate shapes are obtained for $q_2 < 0$ and prolate ones for $q_2 > 0$. The trajectory $S(q_2)$ for which $q_1 = q_3 = q_4 = \cdots = 0$ corresponds, to a good approximation, to the liquid-drop path to fission as demonstrated in Fig. 2. The deformation parameter $q_5$ is chosen in such a way that for a given elongation (triggered by $q_2$) the stiffness of the liquid-drop potential-energy surface with respect the left–right asymmetry parameter $q_3$ is as small as possible. The transformation between the $q_i$ deformation parameters and the Fourier decomposition coefficients $a_i$ is made in the subroutine "*qtoa*".

To obtain the friction and the inertia tensor in the space of the $q_i$ parameters, we first calculate these quantities in the Fourier-parameter space to obtain the $\gamma_{a_i,a_j}$ and $\mathcal{M}_{a_i,a_j}$ tensors and then transform these to the $\{q_i\}$ space according to

$$\begin{aligned} \mathcal{M}_{q_k q_l} &= \sum_{i,j} \mathcal{M}_{a_i a_j} \frac{\partial a_i}{\partial q_k} \frac{\partial a_j}{\partial q_l} , \\ \gamma_{q_k q_l} &= \sum_{i,j} \gamma_{a_i a_j} \frac{\partial a_i}{\partial q_k} \frac{\partial a_j}{\partial q_l} , \end{aligned} \tag{27}$$

a calculation that is carried out at the end of the subroutine "*tcoef* ".

The components of the inertia and friction tensors obtained in this way are shown Fig. 3 along the LD path to fission as function of the relative distance $R_{12}$ between the fragments. One notices that for large values of $R_{12}$ the inertia approaches (as it should) to the reduced mass $\mu$. We also show on the same figure the approximation for the inertia made in Ref. [13].

## 5. Summary

The main purpose of the present work, and of the computer code that comes along with it, is the calculation of the transport functions necessary to perform studies of the nuclear fission process within the dissipative dynamics model. In addition the program evaluates the deformation dependent liquid-drop coefficients which are important ingredients of all macroscopic–microscopic models. The rapidly converging Fourier type parametrization of nuclear shapes used in the program offers a very effective four dimensional (4D) description of the potential-energy surfaces of fissioning nuclei and their fission dynamics.

## Acknowledgements

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## Appendix. Expansion coefficients of the velocity field

The kinetic energy of an ideal incompressible fluid of constant matter density $\varrho_m = 3M/(4\pi R_0^3)$ and velocity field $\vec{v}(\vec{r}\,)$ can be written as

$$T = \frac{1}{2} \rho_m \int_V d^3r \; \vec{v}^{\,2}(\vec{r}\,) , \tag{A.1}$$

with the integration extending over the volume $V$ of the matter distribution. We will show that this kinetic energy can be expressed as a quadratic form in the collective velocities $\dot{s}_i$ associated with the collective coordinates $s_i$ which could be identified in our case as the Fourier shape parameters $a_i$ entering Eq. (6), the non-axiality parameter $\eta$, Eq. (8), or the new collective coordinates defined by (25)

$$T = \frac{1}{2} \sum_{i,j} M_{ij} \dot{s}_i \dot{s}_j , \tag{A.2}$$

where $M_{ij}$ are the components of the collective mass tensor.

In order for Eq. (A.1) to imply Eq. (A.2) it is necessary that the position vector $\vec{r}$ of a fluid element will not depend on the time *explicitly*, but only on the shape of the system, thus implying that its velocity can be written as

$$\vec{v} = \dot{\vec{r}} = \sum_i \frac{\partial \vec{r}}{\partial s_i} \dot{s}_i , \tag{A.3}$$

which directly leads to Eq. (A.2) with

$$M_{ij} = \rho_m \int_V \frac{\partial \vec{r}}{\partial s_i} \cdot \frac{\partial \vec{r}}{\partial s_j} \, d^3r . \tag{A.4}$$

In the general case where no axial symmetry is imposed, the velocity field in cylindrical coordinates $\{\rho, \varphi, z\}$ is written as

$$\vec{v} = \dot{\rho}\, \vec{e}_\rho + \rho\, \dot{\varphi}\, \vec{e}_\varphi + \dot{z}\, \vec{e}_z , \tag{A.5}$$

where $\vec{e}_\rho$, $\vec{e}_\varphi$ and $\vec{e}_z$ denote the unit vectors in $\rho$, $\varphi$ and $z$ directions, respectively.

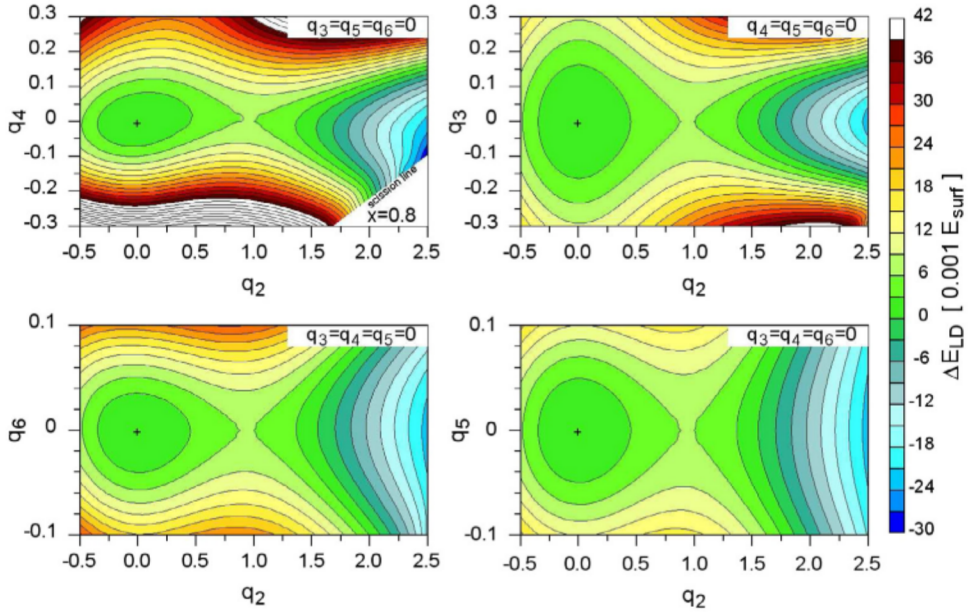


**Fig. 2.** (Colour online) LD potential energy surface in the $(q_2, q_4)$ (top left), $(q_2, q_3)$ (top right), $(q_2, q_6)$ (bottom left) and $(q_2, q_5)$ (bottom right) deformation planes of a nucleus with fissility x=0.8. In each $(q_i, q_j)$ plot, the collective coordinates $q_k$ with $k \neq i, j$ are set to zero.

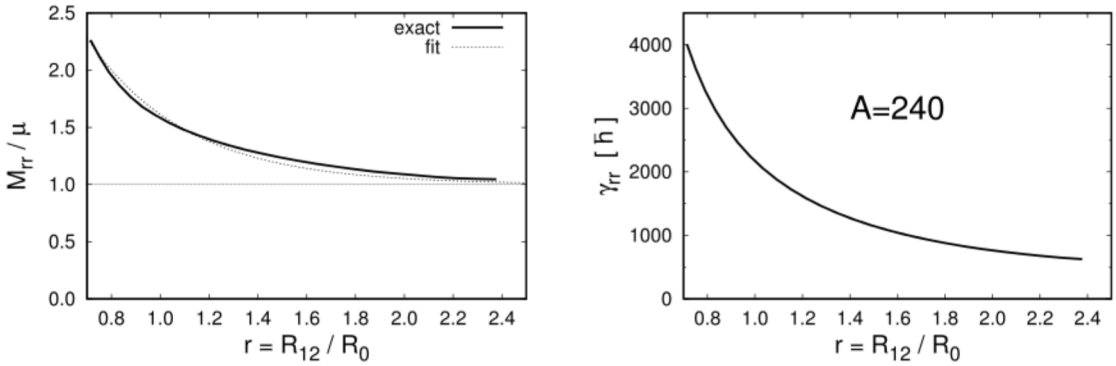


**Fig. 3.** Relative distance component of the irrotational flow inertia (l.h.s) and the wall-friction (r.h.s.) tensors as functions of the relative distance between the mass centres of the nascent fragments. The approximation for the inertia presented in Ref. [13] is shown as the dotted line.

In the axially symmetric case, the Werner–Wheeler approximation consists in supposing that $\dot{z}$ is independent of $\rho$ and that $\dot{\rho}$ depends linearly on $\rho$, i.e.

$$\dot{z} = \mathcal{A}(z, \vec{s}, \dot{\vec{s}}) = \sum_i A_i(z, \vec{s})\, \dot{s}_i \tag{A.6}$$

and

$$\dot{\rho} = \rho\, \mathcal{B}(z, \vec{s}, \dot{\vec{s}}) = \frac{\rho}{\rho_s(z, \varphi)} \sum_i B_i(z, \vec{s})\, \dot{s}_i \,. \tag{A.7}$$

A natural generalization of this approximation to the case of non-axial shapes, as given e.g. by Eq. (7), is the following

$$\begin{aligned} v_x &= (\alpha + \beta)\, x = (\alpha + \beta)\, \rho\, \cos\varphi \\ v_y &= (\alpha - \beta)\, y = (\alpha - \beta)\, \rho\, \sin\varphi \end{aligned} \tag{A.8}$$

where the parameters $\alpha$ and $\beta$ will generally depend on $z$ and the collective coordinates $s_i$. In cylindrical coordinates ($x = \rho\, \cos\varphi$ and $y = \rho\, \sin\varphi$) the $x$ and $y$ components of the velocity field are given by

$$\begin{aligned} v_x &= \dot{x} = \dot{\rho}\, \cos\varphi - \rho\, \dot{\varphi}\, \sin\varphi \\ v_y &= \dot{y} = \dot{\rho}\, \sin\varphi + \rho\, \dot{\varphi}\, \cos\varphi \,. \end{aligned} \tag{A.9}$$

Using the above relations (A.8) and (A.9) we get the following expressions:

$$\begin{aligned} \dot{\rho} &= \rho\, (\alpha + \beta \cos 2\varphi) \\ \dot{\varphi} &= -\beta \sin 2\varphi \,. \end{aligned} \tag{A.10}$$

The velocity field of an ideal fluid should be both source-less and irrotational, i.e.

$$\vec{\nabla} \cdot \vec{v} = 0 \qquad \text{and} \qquad \vec{\nabla} \times \vec{v} = \vec{0} \,. \tag{A.11}$$

The parameters $\alpha$ and $\beta$ can now be evaluated from the divergence-free character of the velocity field, Eq. (A.11), and the condition that the velocities of the wall and of the liquid should be equal at the surface of the body defined by $\rho_s(z, \varphi)$. For the velocity components on the $x$ ($\varphi = 0$) and on the $y$ axis ($\varphi = \pi/2$) one obtains more specifically

$$\begin{aligned} v_x(\rho_s, \varphi = 0, z) &= \dot{\rho}_s(z, \varphi = 0) = \rho_s(z, \varphi = 0)\, [\alpha(z) + \beta(z)] \\ v_y(\rho_s, \varphi = \tfrac{\pi}{2}, z) &= \dot{\rho}_s(z, \varphi = \tfrac{\pi}{2}) = \rho_s(z, \varphi = \tfrac{\pi}{2})\, [\alpha(z) - \beta(z)] \end{aligned} \tag{A.12}$$

where, in the last step, Eq. (A.10) has been used and which directly leads to the following identities for $\alpha(z)$ and $\beta(z)$

$$\begin{aligned}\alpha(z) &= \frac{1}{2}\left[\frac{\dot\rho_s(z,\varphi=0)}{\rho_s(z,\varphi=0)} + \frac{\dot\rho_s(z,\varphi=\frac{\pi}{2})}{\rho_s(z,\varphi=\frac{\pi}{2})}\right]\\ \beta(z) &= \frac{1}{2}\left[\frac{\dot\rho_s(z,\varphi=0)}{\rho_s(z,\varphi=0)} - \frac{\dot\rho_s(z,\varphi=\frac{\pi}{2})}{\rho_s(z,\varphi=\frac{\pi}{2})}\right] .\end{aligned} \tag{A.13}$$

Let us mention here that, in the general case, the velocity components $v_x$ and $v_y$ along the $x$ and $y$ axis as given by Eq. (A.12) are, of course, not the only non-vanishing velocity components, but that, except at the $z$-coordinates where $\partial\rho_s^2(z,\varphi)/\partial z = 0$, the $z$ component $v_z$ of the velocity field is also present. But that is of no concern to us, since the coefficients $\alpha(z)$ and $\beta(z)$ do only enter the definition of the $x$ and $y$ components of the velocity field through Eq. (A.8) and are unambiguously defined through Eq. (A.12).

Using the product ansatz of $\rho_s^2(z,\varphi)$ as given in Eq. (7) one has

$$\frac{\dot\rho_s(z,\varphi)}{\rho_s(z,\varphi)} = \frac{1}{\sqrt{\tilde\rho_s^2(z)f(\varphi)}}\frac{d}{dt}\sqrt{\tilde\rho_s^2(z)f(\varphi)} = \frac{1}{2}\left[\frac{\dot{\tilde\rho}_s^2(z)}{\tilde\rho_s^2(z)} + \frac{\dot f(\varphi)}{f(\varphi)}\right] \tag{A.14}$$

and with the particular definition for $f(\varphi)$ of Eq. (7) one obtains

$$\frac{\dot f(\varphi)}{f(\varphi)} = -\frac{2\dot\eta}{1-\eta^2}\,\frac{2\eta+(1+\eta^2)\cos(2\varphi)}{1+\eta^2+2\eta\cos(2\varphi)} \tag{A.15}$$

which then, together with (A.13), yields

$$\alpha(z) = \frac{1}{2}\frac{\dot{\tilde\rho}_s^2(z)}{\tilde\rho_s^2(z)} = \frac{\dot{\tilde\rho}_s(z)}{\tilde\rho_s(z)} \tag{A.16}$$

and

$$\beta(z) = \frac{\dot\eta}{\eta^2-1} . \tag{A.17}$$

an expression that is only related to the non-axiality parameter $\eta$ and its variation with time, but independent of $z$, something that we shall assume to be generally true in what follows, while the expression for $\alpha(z)$ will be determined below through Eq. (A.11).

Inserting $\alpha$ and $\beta$ as found above into Eq. (A.10) one obtains the following expression for the velocities in a plane of constant $z$

$$\dot\rho = \rho\left[\alpha(z) - \frac{\dot\eta\,\cos(2\varphi)}{(1-\eta^2)}\right] \qquad \text{and} \qquad \dot\varphi = \frac{\dot\eta\,\sin(2\varphi)}{(1-\eta^2)} . \tag{A.18}$$

From the condition $\operatorname{div}\vec v = 0$, Eq. (A.11), one obtains together with (A.8)

$$\frac{\partial v_z}{\partial z} = -\frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} = -2\alpha , \tag{A.19}$$

which corresponds, in the case of axial symmetry, to Eq. (A7) of [10]. Proceeding as in Ref. [10], we suppose that, for an incompressible fluid, the convective time derivative of any fluid element of volume

$$V^*(z;\vec s) = \frac{1}{2}\int_{z_{min}}^{z}\int_0^{2\pi}\rho_s^2(z',\varphi)\,dz' = \pi\int_{z_{min}}^{z}\tilde\rho_s^2(z')\,dz'$$

must vanish:

$$\frac{d}{dt}V^*(z;\vec s) = \dot z\,\frac{\partial}{\partial z}V^*(z;\vec s) + \sum_i \dot s_i\,\frac{\partial}{\partial s_i}V^*(z;\vec s) = 0 ,$$

which can be used to evaluate the $z$-component of the fluid velocity

$$v_z(z) = -\frac{1}{\tilde\rho_s^2(z)}\sum_i \dot s_i\int_{z_{min}}^{z}\frac{\partial\tilde\rho_s^2(z')}{\partial s_i}\,dz' = -\frac{1}{\tilde\rho_s^2(z)}\int_{z_{min}}^{z}\frac{d\tilde\rho_s^2(z')}{dt}\,dz' , \tag{A.20}$$

which means that $v_z$ is linear in the collective velocities $\dot s_i$

$$v_z = \dot z = \sum_i A_i^z(z;\vec s)\,\dot s_i , \tag{A.21}$$

where

$$A_i^z(z;\vec s) = -\frac{1}{\tilde\rho_s^2(z)}\int_{z_{min}}^{z}\frac{\partial\tilde\rho_s^2(z')}{\partial s_i}dz' . \tag{A.22}$$

Using Eq. (A.19) we can evaluate the function $\alpha(z)$

$$\alpha(z) = -\frac{1}{2}\frac{\partial v_z}{\partial z} = -\frac{1}{2}\sum_i\frac{\partial A_i^z}{\partial z}\,\dot s_i = \frac{1}{2\tilde\rho_s^2}\sum_i\left\{\frac{\partial\tilde\rho_s^2}{\partial s_i} + \frac{\partial\tilde\rho_s^2}{\partial z}A_i^z\right\}\dot s_i . \tag{A.23}$$

The two other velocity components that appear in Eq. (A.5) are also linear in the collective velocities

$$\begin{aligned} v_\rho &= \dot\rho = \rho\textstyle\sum_i A_i^\rho(\vec r;\vec s)\,\dot s_i\\ v_\varphi &= \rho\,\dot\varphi = \rho\textstyle\sum_i A_i^\varphi(\vec r;\vec s)\,\dot s_i\end{aligned} \tag{A.24}$$

where our collective coordinates $s_i$ are the Fourier deformation parameters $a_\nu$, and $\eta$. The expansion coefficients of the velocity field are then given by

$$\begin{aligned} A_{a_\nu}^\rho &= \frac{1}{2\tilde\rho_s^2}\left(\frac{\partial\tilde\rho_s^2}{\partial a_\nu} + \frac{\partial\tilde\rho_s^2}{\partial z}A_{a_\nu}^z\right) , & A_\eta^\rho &= -\frac{\cos(2\varphi)}{1-\eta^2} ,\\ A_{a_\nu}^\varphi &= 0 , & A_\eta^\varphi &= \frac{\sin(2\varphi)}{1-\eta^2} ,\\ A_{a_\nu}^z &= -\frac{1}{\tilde\rho_s^2(z)}\int_{z_{min}}^{z}\frac{\partial\tilde\rho_s^2(z')}{\partial a_\nu}dz' , & A_\eta^z &= 0 .\end{aligned} \tag{A.25}$$

The kinetic energy of the liquid can then be written in the form:

$$T = \frac{1}{2}\rho_0\int_V\vec v^{\,2}d^3r = \frac{1}{2}\sum_{i,j}B_{ij}\,\dot s_i\,\dot s_j . \tag{A.26}$$

Inserting Eqs. (A.21) and (A.24) for the velocity components one obtains the following expression for the inertia tensor $B$:

$$\begin{aligned} B_{ij} = \rho_0\textstyle\int_{z_{min}}^{z_{max}}dz\int_0^{2\pi}d\varphi\int_0^{\rho_s(z,\varphi)}\{\rho^2\,[A_i^\rho(z)A_j^\rho(z)\\ +A_i^\varphi(z)A_j^\varphi(z)] + A_i^z(z)A_j^z(z)\}\,\rho\,d\rho .\end{aligned} \tag{A.27}$$

Using the relations:

$$\begin{aligned} &\int_0^{2\pi}\rho_s^2(z,\varphi)d\varphi = 2\pi\tilde\rho_s^2(z) , & &\int_0^{2\pi}\rho_s^4(z,\varphi)d\varphi = 2\pi\tilde\rho_s^4(z)\frac{1+\eta^2}{1-\eta^2} ,\\ &\int_0^{2\pi}\rho_s^2(z,\varphi)\cos(2\varphi)d\varphi = -2\pi\eta , & &\int_0^{2\pi}\rho_s^4(z,\varphi)\cos(2\varphi)d\varphi = -2\pi\tilde\rho_s^4(z)\frac{2\eta}{1-\eta^2} .\end{aligned} \tag{A.28}$$

one obtains the final expressions for the components of the inertia tensor:

$$B_{a_\nu a_\mu} = \frac{\pi}{2}\rho_0\,\frac{1+\eta^2}{1-\eta^2}\int_{z_{min}}^{z_{max}}[\tilde\rho_s^4A_{a_\nu}^\rho A_{a_\mu}^\rho + 2\tilde\rho_s^2A_{a_\nu}^zA_{a_\mu}^z]\,dz , \tag{A.29}$$

$$B_{a_\nu\eta} = \pi\rho_0\,\frac{\eta}{1-\eta^2}\int_{z_{min}}^{z_{max}}\tilde\rho_s^4A_{a_\nu}^\rho\,dz , \tag{A.30}$$

$$B_{\eta\eta} = \frac{\pi}{2}\rho_0\,\frac{1}{1-\eta^2}\int_{z_{min}}^{z_{max}}\tilde\rho_s^4\,dz . \tag{A.31}$$

## References


[1] R.W. Hasse, W.D. Myers, Geometrical Relationships of Macroscopic Nuclear Physics, Spinger-Verlag, Berlin, 1988.
[2] C. Schmitt, B. Nerlo-Pomorska, K. Pomorski, J. Bartel, Phys. Rev. C 95 (2017) 034612.
[3] K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt, Phys. Rev. C 97 (2018) 034319.
[4] K. Pomorski, B. Nerlo-Pomorska, A. Surowiec, M. Kowal, J. Bartel, K. Dietrich, J. Richert, C. Schmitt, B. Benoit, E. de Goes Brennand, L. Donadille, C. Badimon, Nuclear Phys. A 679 (2000) 25.
[5] A.J. Sierk, Phys. Rev. C 96 (2017) 034603.
[6] C. Schmitt, K. Mazurek, P.N. Nadtochy, Phys. Rev. C 97 (2018) 014616.
[7] E. Strumberger, K. Dietrich, K. Pomorski, Nuclear Phys. A 529 (1991) 522–564.
[8] M. Brack, J. Damgaard, A.S. Jensen, H.C. Pauli, V.M. Strutinsky, C.Y. Wong, Rev. Modern Phys. 44 (1972) 320.
[9] J. Blocki, Y. Boneh, J.R. Nix, J. Randrup, M. Robel, A.J. Sierk, W.J. Swiatecki, Ann. Phys., NY 113 (1978) 330.
[10] K.T.R. Davies, A.J. Sierk, J.R. Nix, Phys. Rev. C 13 (1976) 2385.
[11] B. Nerlo-Pomorska, K. Pomorski, J. Bartel, Phys. Rev. C 74 (2006) 034327.
[12] W.D. Myers, W.J. Swiatecki, Nuclear Phys. A 612 (1997) 249.
[13] J. Randrup, S.E. Larsson, P. Moller, S.G. Nilsson, K. Pomorski, A. Sobiczewski, Phys. Rev. C 13 (1976) 229.