Vol. 11 (2018) *Acta Physica Polonica B Proceedings Supplement* No 1

POTENTIAL–ENERGY SURFACES OF HEAVY AND SUPER-HEAVY NUCLEI*

K. Pomorski, B. Nerlo-Pomorska

Uniwersytet Marii Curie-Skłodowskiej, 20-031 Lublin, Poland

J. Bartel, C. Schmitt

IPHC, Université de Strasbourg, CNRS, 67037 Strasbourg, France

(Received December 28, 2017)

Nuclear deformation-energy landscapes are presented in a shape parametrization which allows to describe the vast variety of nuclear deformations through a recently developed Fourier expansion. It is shown that, together with the macroscopic–microscopic model, one is thus able to give a good description of nuclear deformation-energy landscapes. Using a new collective model for the fission process, we are then able to make predictions for the fission-fragment mass yields and kinetic-energy distributions that turn out to reproduce the experimental data quite nicely. Investigating the quantum effects of nuclei in the region of super-heavy nuclei, one finds that these are specially favourable in the region of atomic number $Z=118$, whereas the fission barrier height turns out to be quite large in the region of $Z=110$ which will make the survival probability of these nuclei quite important.

DOI:10.5506/APhysPolBSupp.11.137

1. Introduction

A realistic and efficient description of nuclear shapes has been an everlasting challenge to nuclear theoreticians starting from the early days of nuclear physics, in particular in connection with the large deformations encountered in the fission process. Such a model needs to be able to describe the enormous variety of nuclear deformations ranging from the oblate shapes involved in the transition region, corresponding to the progressive filling of the pf shell, to the very elongated, stretched or more compact shapes encountered in the fission process, including the formation of a neck region

* Presented at the XXIV Nuclear Physics Workshop "Marie and Pierre Curie", Kazimierz Dolny, Poland, September 20–24, 2017.

between the two nascent fission fragments. In the present contribution, we are going to use a Fourier-type decomposition of nuclear shapes that will turn out to be very rapidly converging, and this for any deformation. Such a fast convergence and the resulting low dimensionality of the deformation space are particularly important when performing a variational calculation under the constraint on one or several multipole moments. Section 2 will be devoted to the presentation of that Fourier decomposition of nuclear shapes.

We are going to make use of these shapes in a macroscopic–microscopic model to determine the deformation energies of nuclei from the ground state up to the scission point, where we are particularly interested in a realistic description of fission barriers that determine the survival probability of nuclei. Due to the presence of quantal corrections to the liquid-drop-type behaviour, the fission-fragment mass distributions change dramatically when going from light-to-heavy actinides, evolving from a symmetric to a more asymmetric fission. Making predictions on these fission-fragment mass distributions is a stringent test on the validity of our approach. Section 3 will be devoted to this question. We are going to show that we are not only able to give a fair description of fission-fragment mass distributions, but also on the fission-fragment kinetic energies observed in these reactions.

In this context, we are also particularly interested in nuclei in the region of super-heavy elements ($Z = 105$ and beyond) to investigate their stability against fission or other decay modes, in particular α emission. These questions will be addressed in Section 4.

2. Model

The nuclear potential energy surfaces (PES) that are presented below are determined in a liquid-drop-type approach, where the macroscopic energy is evaluated in the Lublin–Strasbourg Drop (LSD) [1] that contains, in addition to the standard volume, surface and Coulomb contributions, a curvature term (proportional to $A^{1/3}$) and a so-called congruence energy [2]. All these contributions, except for the volume term, carry their deformation dependence. This approach has proven [1] not only to yield excellent nuclear masses, but also to reproduce nuclear fission-barrier heights. Microscopic energy that takes into account the quantal nature of the problem is included through Strutinsky shell corrections, obtained from a Yukawa-folded single-particle potential, while pairing correlations are determined through the BCS approach with a monopole pairing force. In this way, one is able to obtain some quite precise evaluation of the nuclear deformation-energy landscape to a point where one is even able to make predictions about the fission-fragment mass distribution [3].

As already pointed out above, it is essential for a correct description of nuclear deformation-energy surfaces to be able to include the physically relevant deformation degrees of freedom in a way as close as ever possible to the physical reality. For many years, we have used the so-called *Modified Funny Hills* shape parametrization [4], which has proven extremely successful, but that does not allow to test its convergence. Recently, we have proposed a Fourier expansion of the nuclear surface [5] which writes in cylindrical coordinates

$$\frac{\rho_{\rm s}^2(z)}{R_0^2} = \sum_{n=1}^{\infty} \left[a_{2n} \cos\left(\frac{(2n-1)\pi}{2} \, \frac{z-z_{\rm sh}}{z_0} \right) + a_{2n+1} \sin\left(n\pi \, \frac{z-z_{\rm sh}}{z_0} \right) \right] , \quad (2.1)$$

where $\rho_{\rm s}(z)$ is the distance from the symmetry axis to the surface of the nucleus at coordinate z and R_0 the radius of the corresponding spherical shape having the same volume. The extension of the nuclear 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 $\rho_{\rm s}^2(z)$ vanishes, a condition which is automatically satisfied by Eq. (2.1). The shift coordinate $z_{\rm sh}$ is chosen such that the center of mass of the shape is always located at the origin of the coordinate system (see Refs. [3, 5] for a more detailed discussion).

To describe non-axial shapes, one can introduce a non-axiality parameter η that is related to the relative ratio of the half-axis a and b perpendicular to the elongation z axis. Supposing that this parameter is independent of z, non-axial shapes can simply be described by multiplying $\rho_{\rm s}^2(z)$ of Eq. (2.1) by a function $F_\eta(\varphi)$ thus obtaining the distance from the elongation z-axis in the form $\varrho_{\rm s}(z,\varphi)$.

As explained above, it would be nice if one could work with a minimum amount of deformation parameters. Let us say with only 3: one related to the elongation of nucleus (q_2), one to its left–right asymmetry (q_3), and one responsible for the neck-formation (q_4) plus, if necessary, the non-axial deformation (η). This can be achieved be redefining our deformation parameters in such a way that higher order parameters simply vanish along the liquid-drop path to the scission configuration. This is achieved by introducing the following new collective coordinates:

$$\begin{aligned} q_2 &= a_2^{(0)}/a_2 - a_2/a_2^{(0)} \,, \qquad q_3 = a_3 \,, \qquad q_4 = a_4 + \sqrt{(q_2/9)^2 + \left(a_4^{(0)}\right)^2} \,, \\ q_5 &= a_5 - a_3(q_2-2)/10 \,, \quad q_6 = a_6 - \sqrt{(q_2/100)^2 + \left(a_6^{(0)}\right)^2} \,, \end{aligned} \quad (2.2)$$

where the $a_n^{(0)}$ are the expansion coefficients for a sphere. This definition allows to describe even very strongly elongated shapes quite precisely with only 4 deformation parameters (3 in the case of axial symmetry).

As an illustration, we show in Fig. 1 the total energy related to the LSD energy for sphere of the nucleus ^{236}Pu 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 $q_2 \approx 0.75$, again left–right symmetric, a second barrier which is higher than 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 path seems to be deeper than the symmetric one. We thus expect some bimodal fission in ^{236}Pu with an asymmetric fission that dominates.

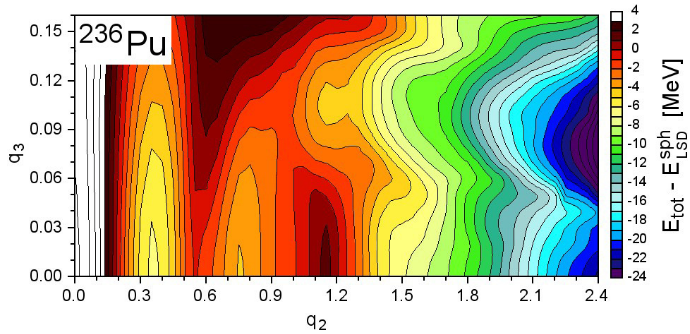

Fig. 1. Potential energy surface in the elongation–mass-asymmetry deformation space minimized with respect to the neck parameter q_4.

3. Deformation-space probability distribution and neck breaking

A quantal system as a fissioning nucleus does not evolve along a given trajectory in deformation space but rather has a certain probability distribution to be located at a given time in a given point in deformation space, characterized in our Fourier shape parametrization by the values of our deformation parameters $\{q_2, q_3, q_4, \cdots\}$. To obtain such a probability distribution, we have to solve the eigenvalue problem of a collective Hamiltonian with deformation-dependent potential and inertia tensor. Considering the fission process to proceed on a time scale that is much longer than the one for the rearrangement of the nucleons inside the nucleus, the eigenfunctions of this collective Hamiltonian can be written in the Born–Oppenheimer approximation in factorized form [6]. For low-energy fission, it is sufficient to use the WKB approximation for the eigenfunction in the fission direction and to consider only the lowest energy eigenstate in the perpendicular direction [7]. It has been shown [9] that the probability $P(q_2; q_3, q_4)$ of finding the nuclear system for a given elongation, characterized by q_2 in a certain point $\{q_3, q_4\}$ in deformation space can then be simply approximated by a normalized Wigner function

$$P(q_2; q_3, q_4) \sim \exp\left[\frac{V(q_2; q_3, q_4) - V_{\rm eq}(q_2)}{E_0}\right] , \qquad (3.1)$$

where $V_{\rm eq}(q_2)$ is the minimum of the potential for given elongation q_2 and E_0 is the zero-point energy treated here as a free parameter. Since the left–right asymmetry parameter q_3 is directly related to the fragment mass distribution, integrating over q_4 will give a probability distribution $\tilde{P}(q_2; q_3)$ that determines the fragment mass yield at given elongation q_2. In order to determine for which set of deformation parameters the scission takes place, we define a neck-breaking probability that will be a function of the neck size $r_{\rm neck}$. Whenever the neck of the nuclear shape becomes narrow enough, *e.g.* of the size of a nucleon or an α particle, there should be a certain probability that the nucleus splits into two pieces. To get some idea on how such a condition could look like in the deformation space of a strongly deformed nucleus, we present in Fig. 2 an energy landscape of the ^{236}Pu nucleus at very large deformation ($q_2 = 2.25$), close to the scission point, where lines of constant neck size (the size of an nucleon and an α particle respectively) are shown in the (q_3, q_4) deformation space.

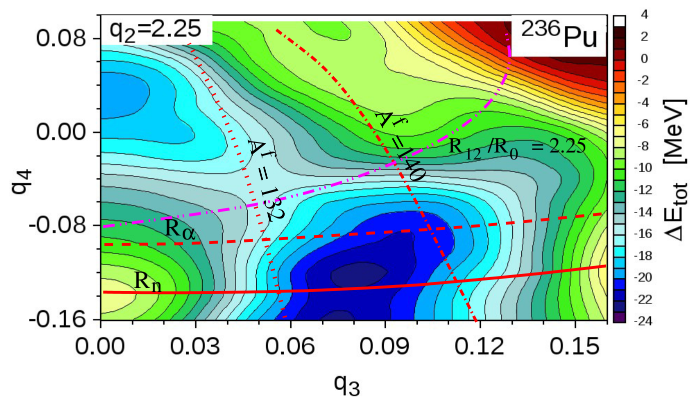

Fig. 2. Total energy relative to the LSD energy for a sphere (ΔE) for the nucleus ^{236}Pu as a function of q_3 and q_4 for an elongation of $q_2 = 2.25$. The distance R_{12} of the nascent fragments given by $2.25R_0$ is represented by the dash-double-dotted line. Dotted and dash-dotted lines show the deformation where the mass of the heavy fragment is equal to 132 and 140 respectively, while solid and dashed lines indicate where the neck is, respectively, of the size of a nucleon or an α particle.

We have tested different neck-breaking probability functions

$$p_{\rm neck} = \begin{cases} \exp\left[-\ln 2 \left(\frac{r_{\rm neck}}{d}\right)^2\right] , & \text{Gauss}\,, \\ \left[\cosh\left\{\ln\left(2+\sqrt{3}\right) \frac{r_{\rm neck}}{d}\right\}\right]^{-1} , & \cosh^{-1}\,, \\ \left[1+\left(\frac{r_{\rm neck}}{d}\right)^2\right]^{-1} , & \text{Lorentz}\,, \end{cases} \tag{3.2}$$

where in all cases d is the half-width of the probability distribution. This function obviously depends on all of the deformation parameters. Convoluting the probability distribution $P(q_2; q_3, q_4)$ with this neck-breaking probability functions yields a fission probability

$$W(q_2, q_3) = \int P(q_2; q_3, q_4)\, p_{\rm neck}(q_2; q_3, q_4)\, {\rm d}q_4\,. \tag{3.3}$$

Such an approach implies that the fission process is spread over some region in the elongation parameter q_2. That, however, means that for given q_2 and mass asymmetry q_3, one has to take into account that the nuclear system might have fissioned at a previous q_2 value, *i.e.* instead of $W(q_2, q_3)$, Eq. (3.3), one has to use the function

$$\tilde{W}(q_2, q_3) = W\left(q_2, q_3\right) \left[1 - \frac{\int_{q_2' \le q_2} W\left(q_2', q_3\right) {\rm d}q_2'}{\int_{{\rm all}\, q_2'} W\left(q_2', q_3\right) {\rm d}q_2'}\right] \tag{3.4}$$

that keeps track of the previous *history* of the evolution towards fission. The final mass yield $Y(q_3)$ will then be given as the sum of all partial ones obtained at different q_2 values

$$Y(q_3) = \frac{\int \tilde{W}(q_2, q_3){\rm d}q_2}{\int \tilde{W}(q_2, q_3){\rm d}q_2{\rm d}q_3}\,. \tag{3.5}$$

It thus turns out that our approach [8] depends on just 2 parameters, the width parameter E_0 of the Wigner function and the width parameter d of the neck breaking probability. That this way to determine the mass yields is reasonable is demonstrated in Fig. 3, where the nuclear energy of ^{236}Pu is shown for a sequence of elongations q_2, ranging from $q_2 = 2.15$ to $q_2 = 2.50$, as a function of the heavy-fragment mass and the neck radius. One can clearly see that for smaller elongations, a mass splitting is energetically favoured where the heavy fragment has a mass close to $A_{\rm h} \approx 136$, while with increasing elongations, the energetically favoured mass region becomes quite broad with, at $q_2 = 2.50$, even 3 minima at masses $A_{\rm h} \approx 124$, 136 and 143. The resulting mass yield is shown, together with the experimental

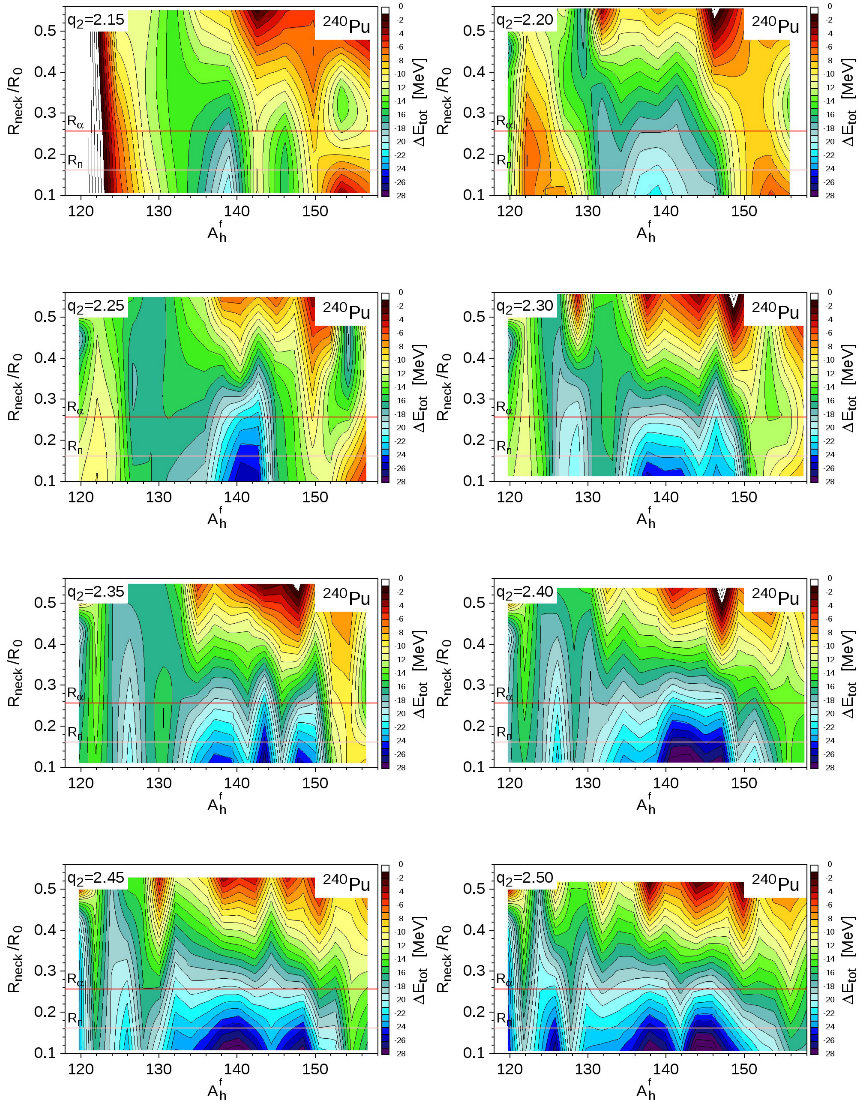

Fig. 3. Total energy of ^{236}Pu as a function of the heavy-mass fragment $A_{\rm h}^{\rm f}$ and the neck radius $R_{\rm neck}/R_0$ for different elongations $q_2 = 2.15$–2.50.

data, for the nucleus ^{240}Pu in Fig. 4. Considering the simplicity of our approach with only 2 adjustable parameters, $E_0 = 1$ MeV and $d/R_0 = 0.15$, one could estimate the reproduction of the experimental data by our model as quite satisfactory. Even though these two parameters have been adjusted to the experimental mass yield of ^{240}Pu, it turns out that the mass yields of other actinide nuclei can be reproduced with a similar quality keeping these parameters fixed.

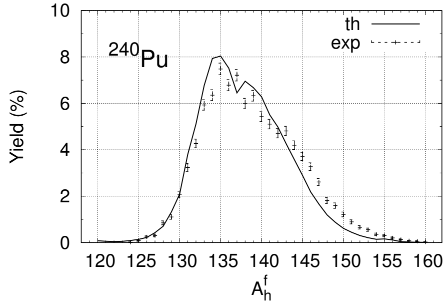

Fig. 4. Comparison between the fission-fragment mass yield of ^{240}Pu obtained in our approach with the experimental data [10].

That we are not only able to reproduce the fission-fragment mass distribution but that their total kinetic energies distribution can also be described with some reasonable accuracy is shown in Fig. 5.

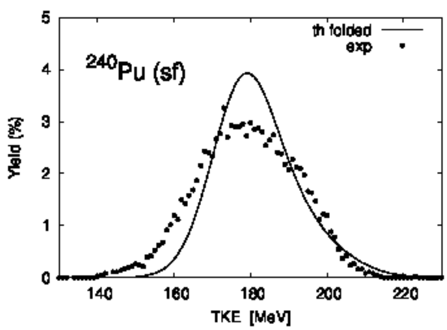

Fig. 5. Comparison between the fission-fragment total kinetic energies (TKE) for ^{240}Pu obtained in our approach with the experimental data from [11].

4. Energy surfaces and survival of super-heavy elements

Our approach should be evidently also applied to the region of super-heavy elements. A first question that needs to be addressed is the one of the probability of forming such nuclei, a probability that will, of course, depend on the quantal corrections deciding whether or not such a nucleus has a chance to be formed and to survive a minimum amount of time. We have, therefore, calculated the nuclear deformation energies (including, of course, everywhere these quantal corrections) for nuclei in the whole region between plutonium ($Z = 94$) and $Z = 126$. Figure 6 shows the total energy landscapes related to the LSD energy for the sphere as a function of the elongation q_2 and the asymmetry parameter q_3 for the nuclei $^{292-296}_{118}$Og and $^{296-300}$120.

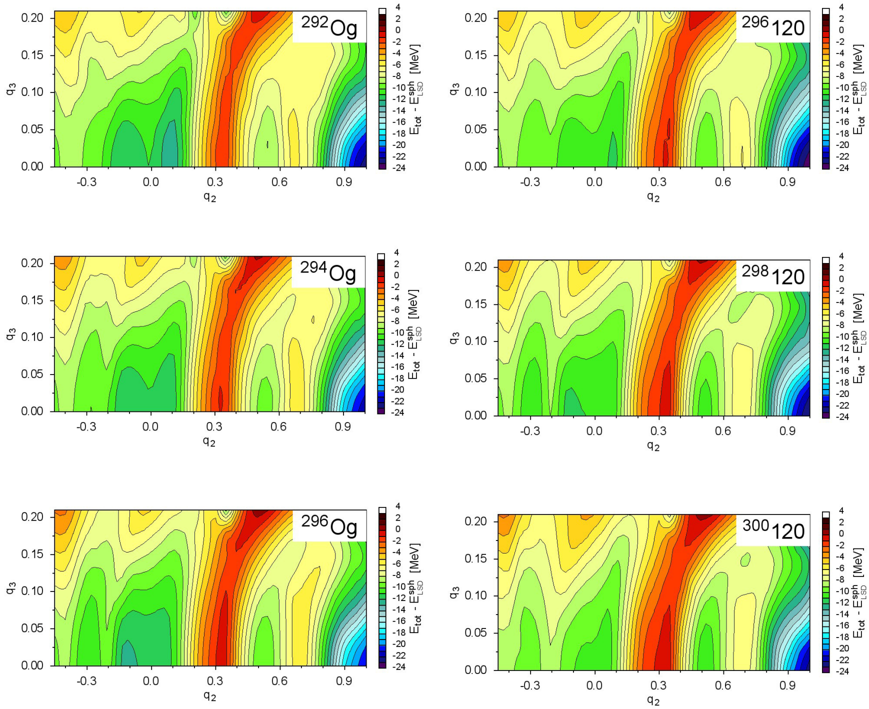

Fig. 6. Total energy landscapes in the (q_2, q_3) deformation plane for the nuclei ${}^{292-296}_{118}$Og and ${}^{296-300}$120 minimized with respect to q_4.

It appears that these nuclei have an essentially spherical ground-state deformation and will have to overcome a fairly high potential barrier to undergo fission which, of course, can contribute to their stability.

In order to get a much broader view on the possible stability of the nuclei in that whole region of the nuclear chart, we show in Fig. 7 the microscopic energy corrections in the ground state of these nuclei. One can clearly see that these shell and pairing energy corrections are particularly large (favourable) in the region around $Z = 116$ (livermorium) with a mass number of about $A \approx 285$. We have also determined the fission-barrier heights of all these nuclei. Here, these barrier heights seem to be most important for nuclei around ${}^{270}_{108}$Hs. However, such a nucleus cannot only undergo spontaneous fission, but also decay through α emission. We have, therefore, also determined the Q_α values and the α-decay half-lives $T^{\alpha}_{1/2}$ for all of the nuclei in that same mass region, which are displayed in Fig. 8. A comparison with the available experimental Q_α values with an r.m.s. deviation of only 0.51 MeV shows that our estimates are, indeed, quite satisfactory.

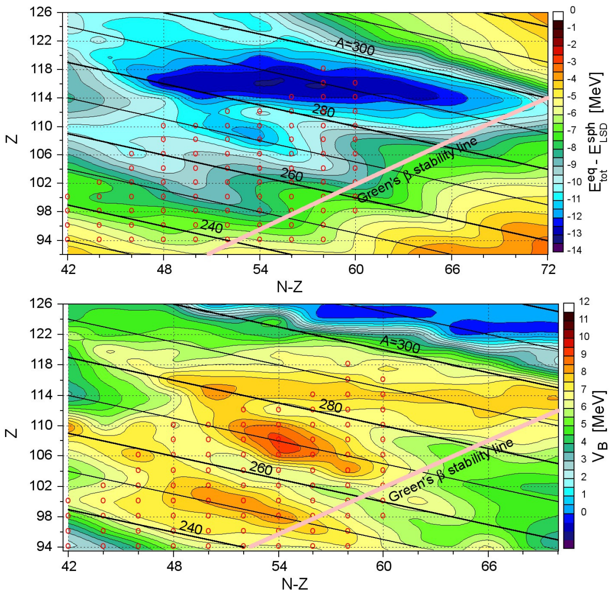

Fig. 7. Microscopic energy corrections in the ground states of the nuclei in the super-heavy region (top) and fission barrier heights (bottom).

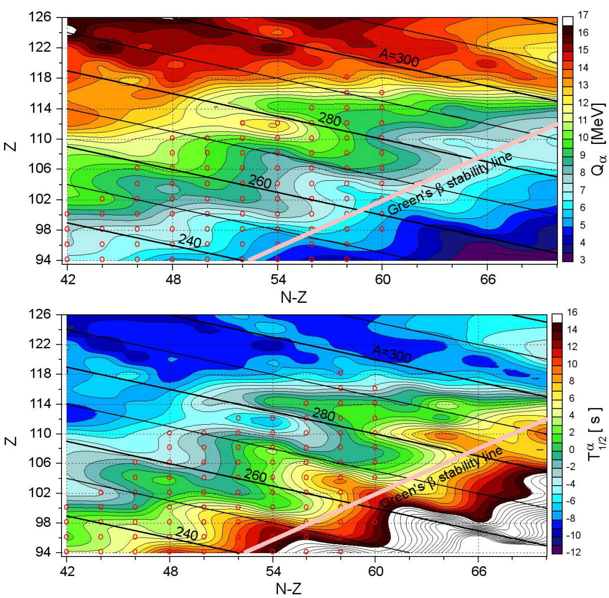

Fig. 8. Q_α values (top) and α-decay half-lives $T^{\alpha}_{1/2}$ (bottom) for the region of super-heavy elements.

5. Conclusions

A new very rapidly converging Fourier expansion of nuclear shapes has been introduced that turns out to yield a good description of nuclear deformation-energy surfaces up to very large deformations like they are encountered in the fission process. We have shown that with a clever definition of our deformation coordinates, one is able to work effectively in a 3-dimensional deformation space that is represented by elongation, mass-asymmetry and neck degrees of freedom. The forth coordinate, *viz.* triaxiality, influences the potential energy surfaces of investigated nuclei at small deformations only, at larger elongation its effect is negligible. Assuming a Wigner-type probability distribution of neck and asymmetry degrees of freedom and a neck-breaking probability which depends on the neck size, one is able to predict fission-fragment mass and total kinetic-energy distributions quite successfully. We have finally extended our analysis to the region of super-heavy nuclei and give predictions on quantum shell and pairing corrections, fission-barrier heights, Q_α values and α-decay half-lives $T^{\alpha}_{1/2}$ for the whole region of super-heavy elements.

This work has been partly supported by the Polish–French COPIN-IN2P3 collaboration agreement under project number 08-131 and by the National Science Centre, Poland (NCN) grant No. 2016/21/B/ST2/01227.

REFERENCES

[1] K. Pomorski, J. Dudek, *Phys. Rev. C* **67**, 044316 (2003).

[2] P. Meller, J.R. Nix, W.D. Myers, W.J. Swiatecki, *At. Data Nucl. Data Tables* **59**, 185 (1995).

[3] C. Schmitt, K. Pomorski, B. Nerlo-Pomorska, J. Bartel, *Phys. Rev. C* **95**, 034612 (2017).

[4] K. Pomorski, J. Bartel, *Int. J. Mod. Phys. E* **15**, 417 (2006).

[5] K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt, *Acta Phys. Pol. B Proc. Suppl.* **8**, 667 (2015).

[6] M. Born, J.R. Oppenheimer, *Ann. Phys.* **389**, 457 (1927).

[7] B. Nerlo-Pomorska, K. Pomorski, F.A. Ivanyuk, *Acta Phys. Pol. B Proc. Suppl.* **8**, 659 (2015).

[8] K. Pomorski, F.A. Ivanyuk, B. Nerlo-Pomorska, *Eur. Phys. J. A* **53**, 59 (2017).

[9] K. Pomorski, B. Nerlo-Pomorska, J. Bartel, C. Schmitt, *Eur. Phys. J. Conf. Proc.*, in print.

[10] L. Dématté *et al.*, *Nucl. Phys. A* **617**, 331 (1997).

[11] C. Wagemans *et al.*, *Phys. Rev. C* **30**, 218 (1984).