POTENTIAL ENERGY SURFACES OF MERCURY UP TO URANIUM ISOTOPES IN THE 4D FOURIER SHAPE PARAMETRISATION* **

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The potential energy landscapes of Hg–U nuclei were calculated within the macroscopic–microscopic method with a Fourier nuclear shape parametrisation and the Lublin–Strasbourg Drop for the macroscopic energy. Microscopic corrections based on the Yukawa folded single-particle potential were obtained with the Strutinsky shell-correction method and the BCS approximation. The energy landscapes of even–even isotopes of Hg, Po, Ra and U were analysed in a 4-dimensional deformation space and projected onto the quadrupole–octupole plane. Extrema, ridges and valleys were localized and the electric quadrupole moments in these minima were evaluated. A comparison with the experimental data for the ground state is shown for the Hg isotopes.

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1. Introduction

The detailed knowledge of the potential energy surfaces (PES) of nuclei is necessary to understand many nuclear properties in the ground as well as in isomeric states, but also fission barriers height and the path to fission. It was shown [1] that the predictive power of the PES landscape depends on the parametrisation of the nuclear shape, the number of collective coordinates, and the method used to calculate the potential energy. In our case, this is the 4-dimensional (4D) Fourier parameters space [2] and the macroscopic–microscopic model with the Lublin–Strasbourg Drop (LSD) [3] and the Strutinsky shell correction method [4]. Pairing correlations are taken into account within the BCS theory [5] using an approximate particle number projection [6]. Selected results for even–even nuclei between Hg and U are presented in the following.

2. Fourier expansion of deformed nuclear shapes

The nuclear shape parametrisation based on a Fourier expansion [2] of the profile function $\rho_s^2(z)$ in cylindrical coordinates is used

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

with the condition $\rho_s(z_{\rm sh} - z_0) = \rho(z_{\rm sh} + z_0) = 0$ which is automatically satisfied by Eq. (2.1). The shift coordinate $z_{\rm sh}$ ensures that the mass centre of the nucleus is located in the origin of the coordinate system. The parameters a_2, a_3, a_4 are related to the elongation, left–right asymmetry, and neck degree of freedom, respectively. The length of the nucleus is $2z_0$. Volume conservation yields the relation: $z_0/R_0 = c = \pi/(a_2 - a_4/3 + a_6/5 - \ldots)$. The elongation parameter c is equal to unity for a sphere, smaller than 1 for oblate, and larger than 1 for prolate shapes. For triaxial shapes, we assume, in addition, that the cross-section perpendicular to the z-axis is of ellipsoidal form with the half-axises a and b, such that $\pi ab = \pi\rho^2$, thus ensuring volume conservation. The parameter $\eta = (a - b)/(a + b)$ defines the nonaxiality of the shape. This Fourier parametrisation allows to take an arbitrary number of dimensions into account, but is so rapidly convergent that only four deformation parameters (three Fourier plus one non-axiality parameter) are sufficient to provide a good description of the considered nuclei.

The liquid drop (LD) paths to fission correspond to decreasing values of $a_2 > 0$ and growing negative values of a_4. That is why it is more convenient to introduce effective collective coordinates which ensure a more convenient presentation of the PES and, as shown below, a better convergence:

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

where $a_0^{(0)} = 1.03205$ and $a_4^{(0)} = -0.03822$ $a_6^{(0)} = 0.00826$ are the values of the Fourier parameters for the spherical shape [2]. q_2 describes nuclear elongation, q_3 — octupole deformation, q_4 — neck parameter, q_5, q_6, ...— higher order modes.

3. Results

The PES of 100 even–even nuclei between Hg and U have been determined, as explained above, in the framework of the macroscopic–microscopic method with the LSD mass formula, the Strutinsky method [4] and the BCS theory [5, 6]. Single-particle energy levels were obtained within a deformed Yukawa-folded potential [7].

In what follows, PESs are presented on the (q_2, q_3) plane after minimization, in every mesh point, with respect to the q_4, η coordinates. The energy has always been displayed relative to the LSD energy of the corresponding spherical nucleus.

The 4D energy landscapes for about 100 even–even isotopes between Pt ($Z = 78$) and Pu ($Z = 94$) were thus calculated as a function of elongation, left–right asymmetry, neck formation, and non-axiality. Some first results for Th isotopes were already presented in Ref. [8].

Here, we show the PESs of Hg, Po, Ra, and U nuclei. The ground state minima and shape isomers are identified, and their quadrupole moments calculated. The paths to fission are analysed.

In Figs. 1–4, the deformation energies for respectively 8 isotopes of Hg, Po, Ra and U are shown as a function of elongation (q_2) and left–right asymmetry (q_3), after minimization with respect to non-axiality (η) and neck parameter (q_4).

When looking at the Hg chain in Fig. 1, one notices that, for the neutron deficient isotopes $^{178-182}$Hg, the potential energy valley corresponds at the largest elongations ($q_2 > 2$) to a reflection asymmetric partition of the nucleus with the heavy-fragment mass around 100–110 depending on the mass number of the isotope, which is in a good agreement with the experimental data [10]. Nevertheless, it is important to emphasize that a clear evolution of the static fission path occurs with increasing Hg mass number. Indeed, for the lightest $^{178-182}$Hg isotopes, an asymmetric valley appears already at

$q_2 \approx 1$, while the minimum energy path evolves through a symmetric splitting for a sizeable part, and to an asymmetric partition only at the very last stage beyond $q_2 \approx 1.7$.

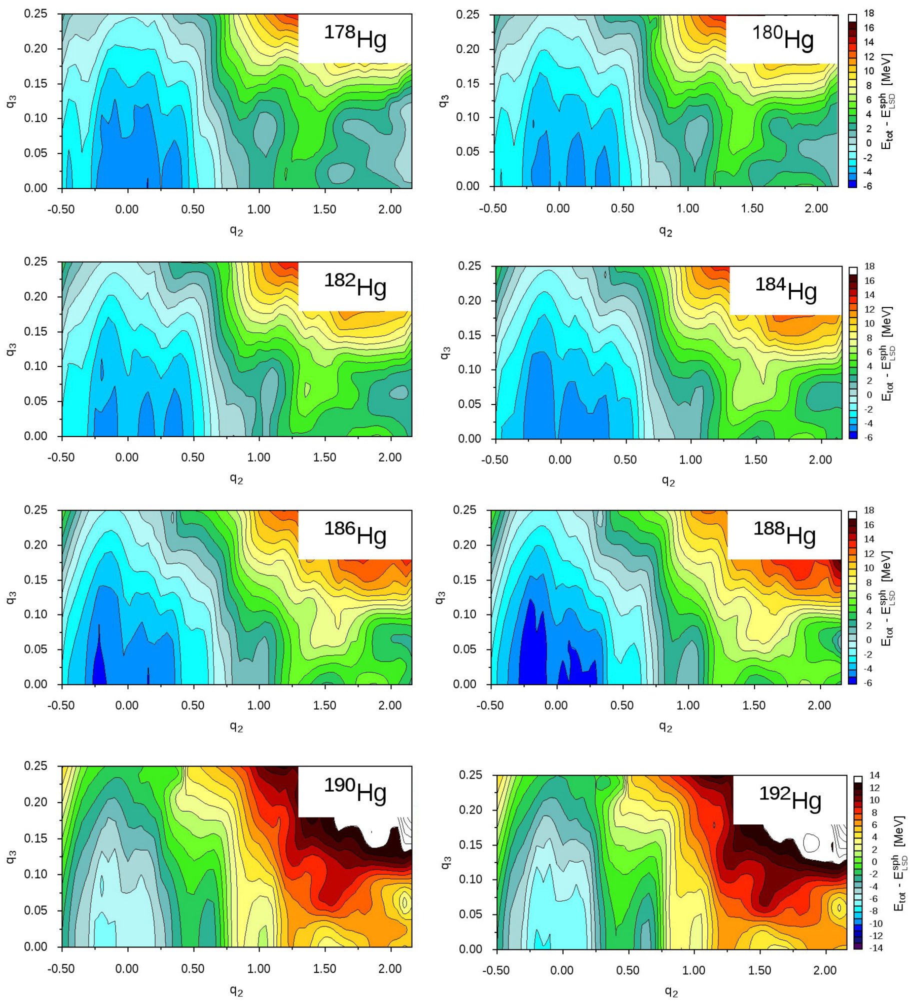

Fig. 1. Deformation energy landscapes on the (q_2, q_3) plane for Hg isotopes.

Considering now the Po isotopic chain in Fig. 2, investigated already in Ref. [11] in the Modified Funny Hills parametrisation [9], one concludes that the potential energy landscapes suggest a coexistence of symmetric and asymmetric fission for the most neutron deficient isotopes, whereas only symmetric fission is expected for the heavier isotopes. Such a prediction is fully in line with recent experimental data [12, 13].

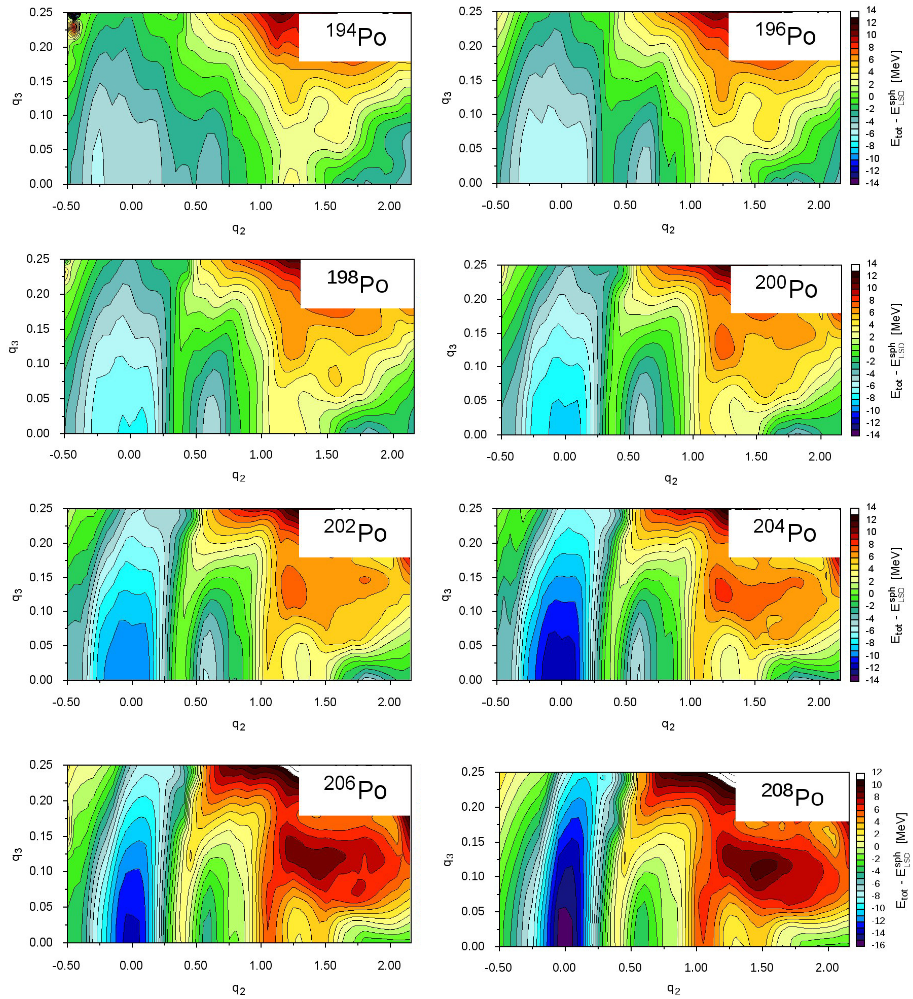

Fig. 2. Deformation energy landscapes on the (q_2, q_3) plane for Po isotopes.

The survey of the Ra chain in Fig. 3 shows that the path to fission corresponding to the minimum energy is reflection-symmetric for all light isotopes. However, an asymmetric valley progressively develops with increasing mass number which competes with the symmetric splitting around ^{222}Ra, and which finally becomes the favoured fission configuration for still heavier Ra isotopes. This evolution is also in a good agreement with experimental data (see [14] and references therein).

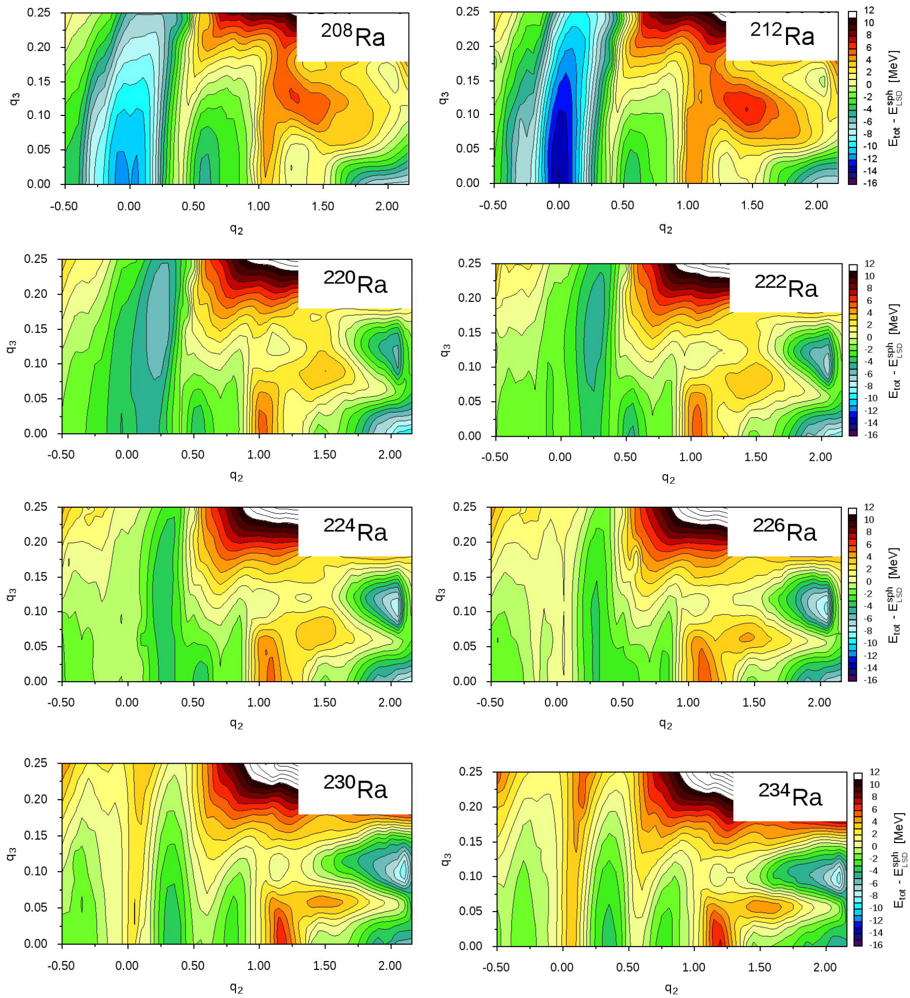

Fig. 3. Deformation energy landscapes on the (q_2, q_3) plane for Ra isotopes.

Finally, regarding the U chain in Fig. 4, a very pronounced asymmetric valley dominates for most of the chain, except the very lightest isotopes. This conjecture is, again, in an agreement with so far available experimental information [14].

More quantitative predictions of fission-fragment mass distributions will, of course, require to go beyond the static picture employed here, and to include dynamical effects. The work in this direction is on our agenda.

The calculated fission barriers in the investigated region are quite massive. We have observed, in addition, that particularly between Po and Th, the inclusion of shell effects produces local minima which correspond to

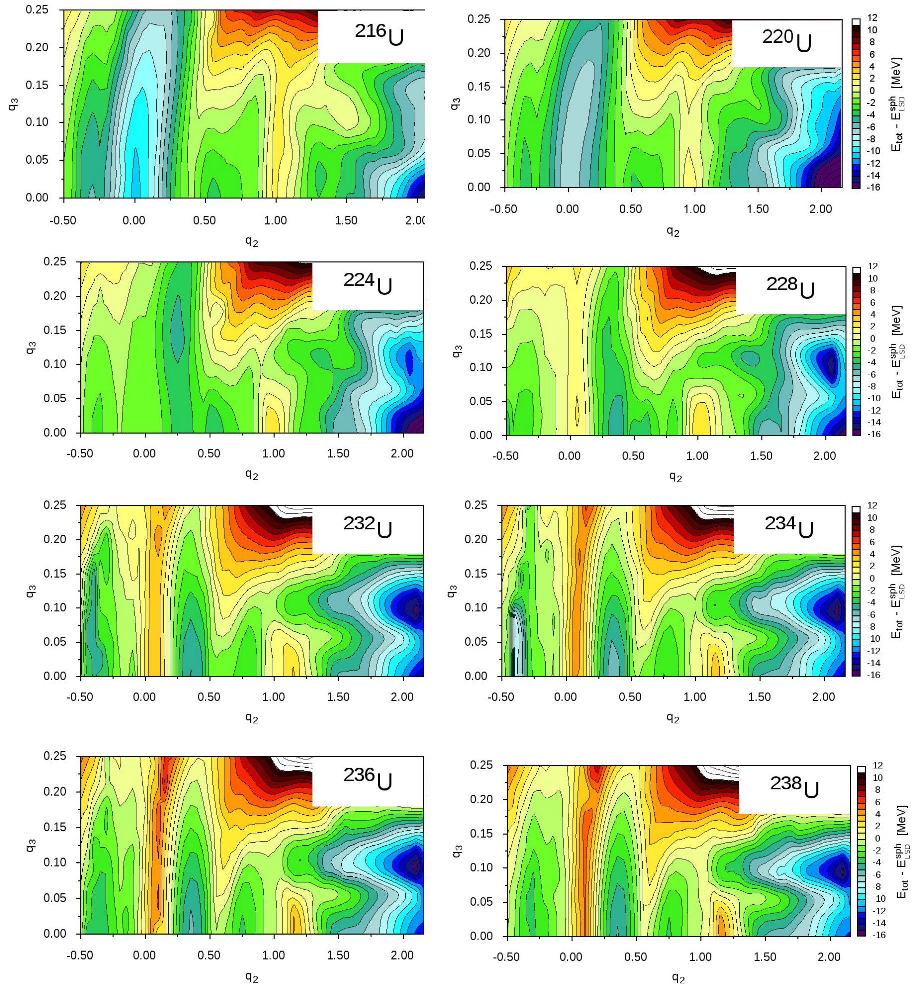

Fig. 4. Deformation energy landscapes on the (q_2, q_3) plane for U isotopes.

super- and hyper-deformed shapes. Several shape isomers are thus predicted in our calculations. An experimental investigation, and possible confirmation of these predictions would ideally involve the use of a proton beam impinging on a suitably target in order to produce a compound system with a limited angular momentum.

The quadrupole moments in the PES minima were evaluated. As an example, the electric quadrupole moments for the Hg isotopic chain are presented in Fig. 5. Experimental data for such exotic shapes in this region would be highly desired.

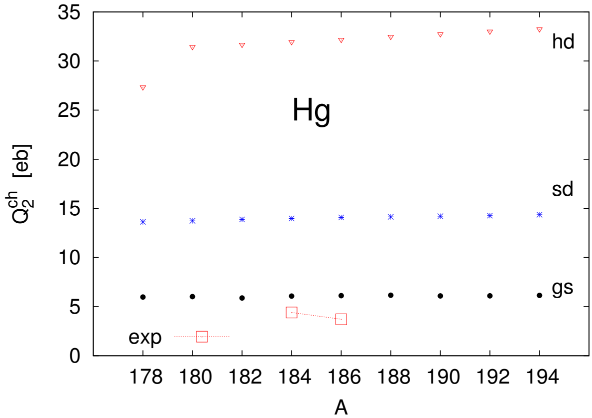

Fig. 5. Electric quadrupole moments $Q_2^{\rm ch}$ for the ground state (gs), super-deformed (sd) and hyperdeformed (hd) isomeric minima along the Hg isotopic chain. Experimental data for the ground state are also shown [15].

4. Summary

Within a macroscopic–microscopic model based on the LSD mass formula, Yukawa-folded single-particle levels, and using a recently developed Fourier shape parametrisation, the potential energy landscapes computed in a 4-dimensional deformation space have been calculated for around 100 isotopes between Pt and Pu. Some of the aspects which can be discussed through a mere analysis of these landscapes are illustrated here for Hg–U elements. A preliminary study of the most probable fission paths, and their evolution with Z and N, is found to match experimental observations. The approach further predicts the existence of several strongly deformed shape isomers in the Pt $\to$ Pu region, including the debated third minimum in heavy actinides. As an example, the electric quadrupole moments for Hg isotopes are given, and await a comparison with experiment.

The above results should be understood as a pilot investigation, aimed to demonstrate the potential and power of the approach.

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