Fission Fragment Mass Distributions of Plutonium Isotopes

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Abstract

Using the potential energy surfaces (PES) calculated within the macroscopic-microscopic model [1, 2], and a phenomenological cranking-type inertia tensor [4], the fragment mass distributions obtained in low-energy fission of light actinides is evaluated in a quantum mechanics framework by solving the eigenvalue problem of a 3-dimensional collective Hamiltonian [5]. Using the eigenstates of this Hamiltonian a distribution probability is defined with the mass asymmetry, neck and elongation degrees of freedom. It allows to introduce a neck-dependent fission probability [6] used to evaluate the mass yields from the distribution probability at different elongations of the fissioning nucleus. The asymmetric valleys in the theoretical PES nicely correspond to the measured mass distributions of fission fragments.

Introduction

The shape-profile function of a fissioning nucleus is expanded in a Fourier series [2, 3]:

$$\frac{\rho_s^2(z,\varphi)}{R_0^2} = \sum_{n=1}^{\infty}\left[a_{2n}\cos\left(\frac{(2n-1)\pi}{2}u\right) + a_{2n+1}\sin\left(\frac{2n\pi}{2}u\right)\right] , \qquad (1)$$

where $u = \frac{z-z_{sh}}{z_0}$ and $z_0 = R_0 c$. The shift of coordinate z_{sh} ensures that the centre of mass is located at the origin of the coordinate system, while the volume conservation condition gives the relation between the elongation of nucleus c and the Fourier expansion coefficients $\pi/(3c) = \sum_{n=1}^{\infty}(-1)^{n-1}a_{2n}/(2n-1)$.
The LD path to fission goes towards smaller a_2 and larger negative values of a_4, so it is convenient to introduce physically more intuitive collective coordinates which ensure an optimal presentation of the potential energy landscape:

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

where $a_2^0 = 1.03205$, $a_4^0 = -0.03822$, and $a_6^0 = 0.00826$ are the expansion coefficients of a sphere. In these coordinates the collective Hamiltonian has the following form:

$$\widehat{H}_{coll} = -\frac{\hbar^2}{2}\sum_{i,j}|M|^{-1/2}\frac{\partial}{\partial q_i}|M|^{-1/2}M_{ij}^{-1}(\{q_i\})\frac{\partial}{\partial q_j} + V(\{q_i\}) , \qquad (3)$$

where $M_{ij}(\{q_i\})$ and $V(\{q_i\})$ denote the inertia tensor and the potential energy, respectively and $|M| = \det(M_{ij})$. The eigenproblem of this Hamiltonian is solved in the Born-Oppenheimer approximation (BOA) in which one assumes that the motion towards fission is much slower than the one in the two other collective coordinates. It means that the eigenfunction of $\widehat{H}_{coll}$ can be written in in product form

$$\Psi_{nE}(q_2,q_3,q_4) = u_{nE}(q_2)\varphi_n(q_3,q_4;q_2) . \qquad (4)$$

Here $u_{nE}(q_2)$ is the wave function for the fission mode and φ_n are the eigenfunctions of the Hamiltonian which describes the collective motion perpendicular to the fission mode.
Using the above relations one can write the eigenvalue equation of the fission mode Hamiltonian in the following form:

$$\left(\hat{T}_{fis} + e_n(q_2)\right) u_{nE}(q_2) = E\, u_{nE}(q_2) . \qquad (5)$$

where the energy $e_n(q_2)$ defines the fission potential for different channels, corresponding to excitations perpendicular to the fission mode. In the following we shall take only the lowest energy channel. So, the probability of finding of a nucleus, for a given value of q_2, in a defined (q_3, q_4) point is equal to

$$|\Psi(q_3,q_4;q_2)|^2 = |u_{0E}(q_2)|^2|\varphi_0(q_3,q_4;q_2)|^2 = |\varphi_0(q_3,q_4;q_2)|^2 \qquad (6)$$

The probability distribution integrated over q_4

$$w(q_3;q_2) = \int |\Psi(q_3,q_4;q_2)|^2 dq_4 , \qquad (7)$$

is directly related to the fragment mass yield at given elongation q_2. Depending on the neck radius, a fissioning nucleus has to make its choice "*to fission or not to fission*". When it *decides for fission* it would leave the phase-space of collective coordinates. Following Ref. [6] we assume the neck-rupture probability P in the form:

$$P(q_3,q_4,q_2) = \frac{k_0}{k}P_{neck}(\kappa) , \qquad (8)$$

where k is the momentum in the direction towards fission (or simply the velocity along the elongation coordinate q_2), while $\kappa = \kappa(q_3,q_4,q_2)$ is the deformation dependent relative neck size. The scaling parameter k_0, plays no essential role, and will disappear from the final expression of the mass distribution, once normalized. The geometry dependent part of the neck breaking probability is taken in the form of a Gauss function (see also [6]):

$$P_{neck}(\kappa) = e^{\kappa^2/d^2} , \qquad (9)$$

what corresponds to the concept of a diffused scission line. The parameters $d \approx 0.165$ fixed by comparing the theoretical fission fragment mass distribution of ^{242}Pu with the experimental data [12].
The momentum k which appears in the denominator of Eq. (8) has to ensure that the probability depends on time in which one crosses the subsequent intervals in q_2 coordinates: $\Delta t = \Delta q_2/v(q_2)$, where $v(q_2) = \hbar k/\overline{M}(q_2)$ is the velocity towards fission. The value of k depends on the difference $E - V(q_2)$ and on the part of the collective energy which is converted into heat Q:

$$\frac{\hbar^2 k^2}{2\overline{M}(q_2)} = E_{kin} = E - Q - V(q_2) . \qquad (10)$$

The fission probability w at q_2 and q_3 will be given by the integral:

$$w(q_3,q_2) = \int_{q_4} |\Psi(q_3,q_4;q_2)|^2 P(q_3,q_4,q_2)\, dq_4 . \qquad (11)$$

Such an approach means that the fission process should be spread over some region of q_2 and that for given q_2 at fixed mass asymmetry one has to take into account the probability to fission at previous q_2 points. i.e. one has to replace $w(q_3,q_2)$ by

$$w'(q_3,q_2) = w(q_3,q_2)\left(1 - \frac{\int_{q_2'\le q_2} w(q_3,q_2')\,dq_2'}{\int w(q_3,q_2')\,dq_2'}\right) . \qquad (12)$$

The mass yield will be the sum of all partial yields at different q_2:

$$Y(q_3) = \frac{\int w'(q_3,q_2)\,dq_2}{\int w'(q_3,q_2)\,dq_2\,dq_3} . \qquad (13)$$

As it is seen from (13) the scaling factor k_0 in the expression for P, Eq. (8), has vanished and does not appear any more in the definition of the mass yield. Our model will thus only have one adjustable parameters d, that appears in the neck-breaking probability (9).

Deformation energies

The potential energy surfaces are calculated within the macroscopic-microscopic model using the Lublin-Strasbourg-Drop (LSD) for the macroscopic part, while the microscopic part was evaluated as the sum of the Strutinsky shell [8] and pairing [9] correction obtained using the single-particle energies of the Yukawa-folded Hamiltonian [10, 11].

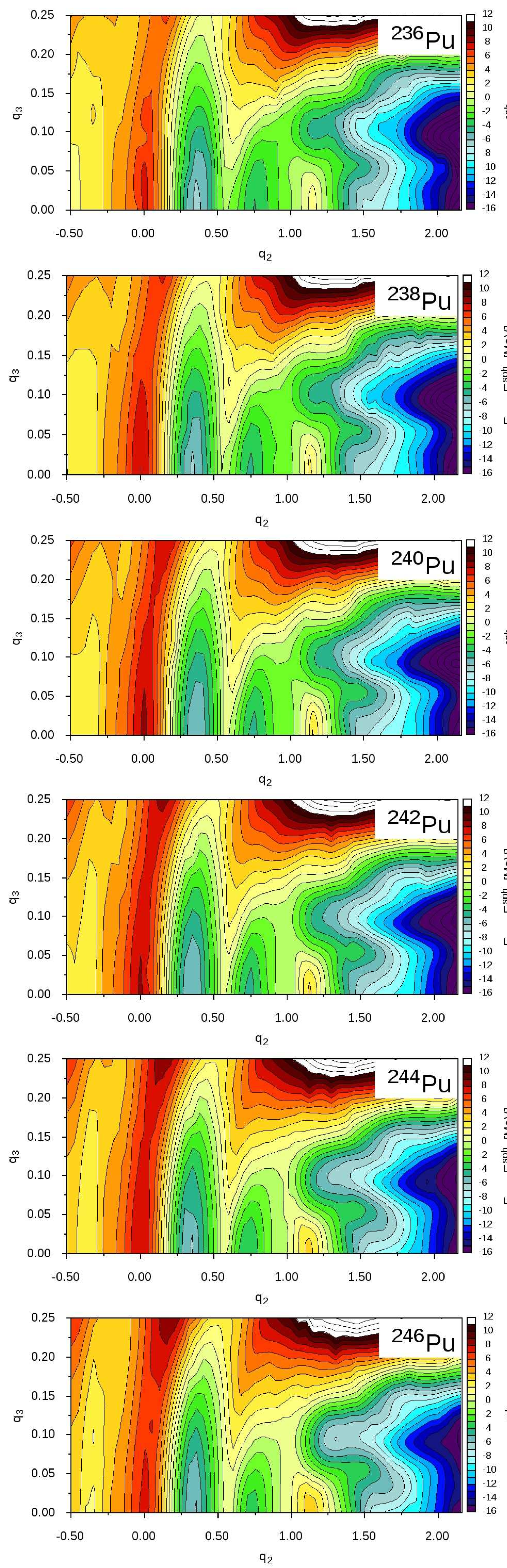

FIGURE 1: Potential energy surfaces Pu isotopes on the (q_2, q_3) plane.

The deformation energy landscapes on the q_2, q_3 plane of $^{236-246}$Pu isotopes are shown in Fig.1. Each point of the maps was minimized with respect q_4. At large elongations q_2 pronounced valleys corresponding to asymmetric fission ($q_3 \neq 0$) are visible. The cross-sections of these maps at elongation $q_2 = 2.05$ are presented in Fig. 2 on the plane (A_f, q_4), where A_f is the mass-number of the heavier fragment. In each map one can see two minima: a deeper asymmetric one around $A_f = 140$ and the other corresponding to symmetric fission. These predictions are in line with the experimental fission yields shown in Fig. 3 [12].
Our model can be still simplified if instead of the square of the collective wave function (6) one uses the Wigner function:

$$w(q3,q4;q2) \sim \exp\left\{-\frac{V(q_3,q_4;q_2) - V_{eq}(q_2)}{E_0}\right\} \qquad (14)$$

where $V_{eq}(q_2)$ is the potential minimum for a given elongation q_2 and E_0 is the zero-point energy treated here as a free parameter.

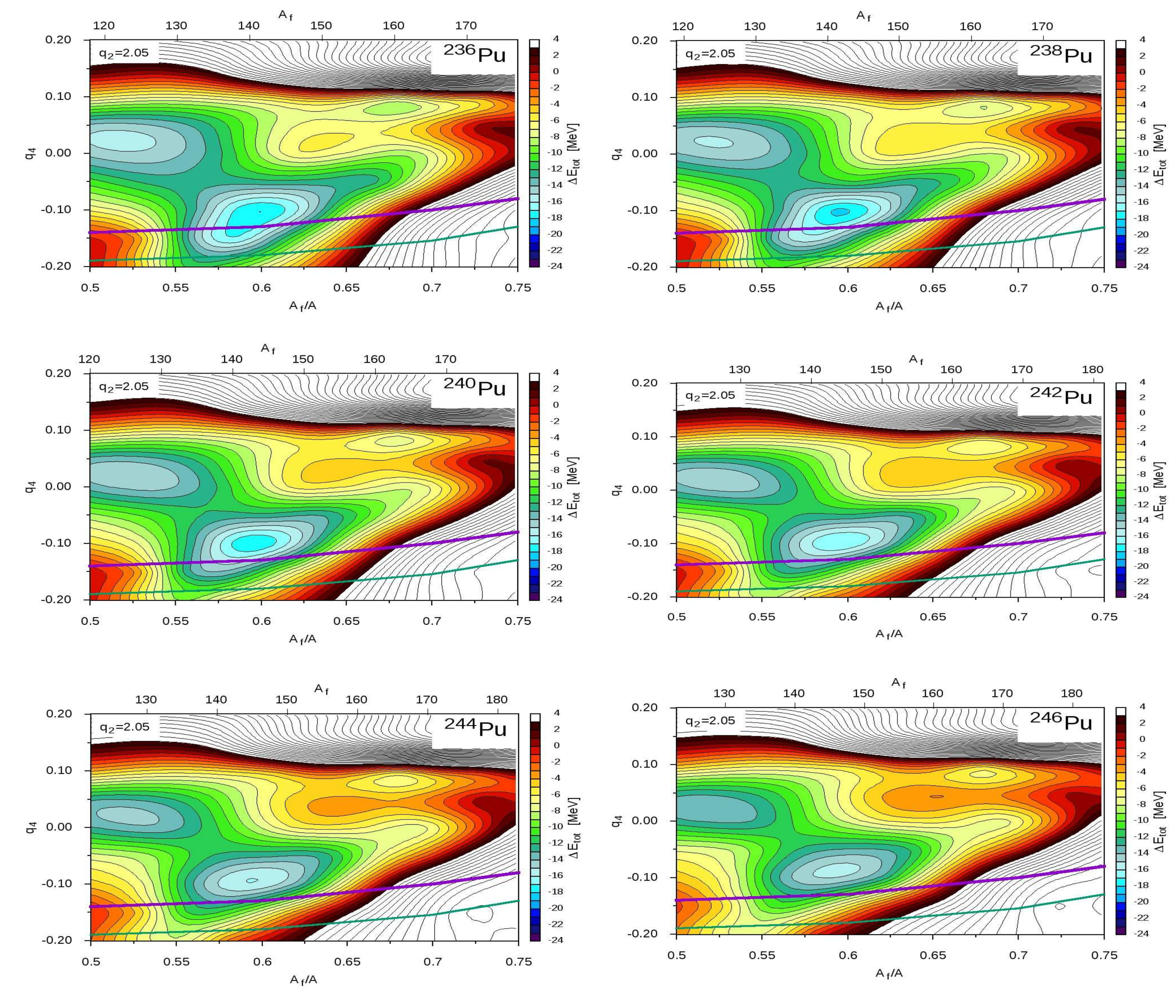

FIGURE 2: Potential energy surfaces for $^{236-246}$Pu isotopes on the (q_3, q_4) plane at elongation $q_2 = 2.05$. The thick violet line corresponds to the neck radius r_{nk}=2 fm while the green one to r_{nk}=1 fm .

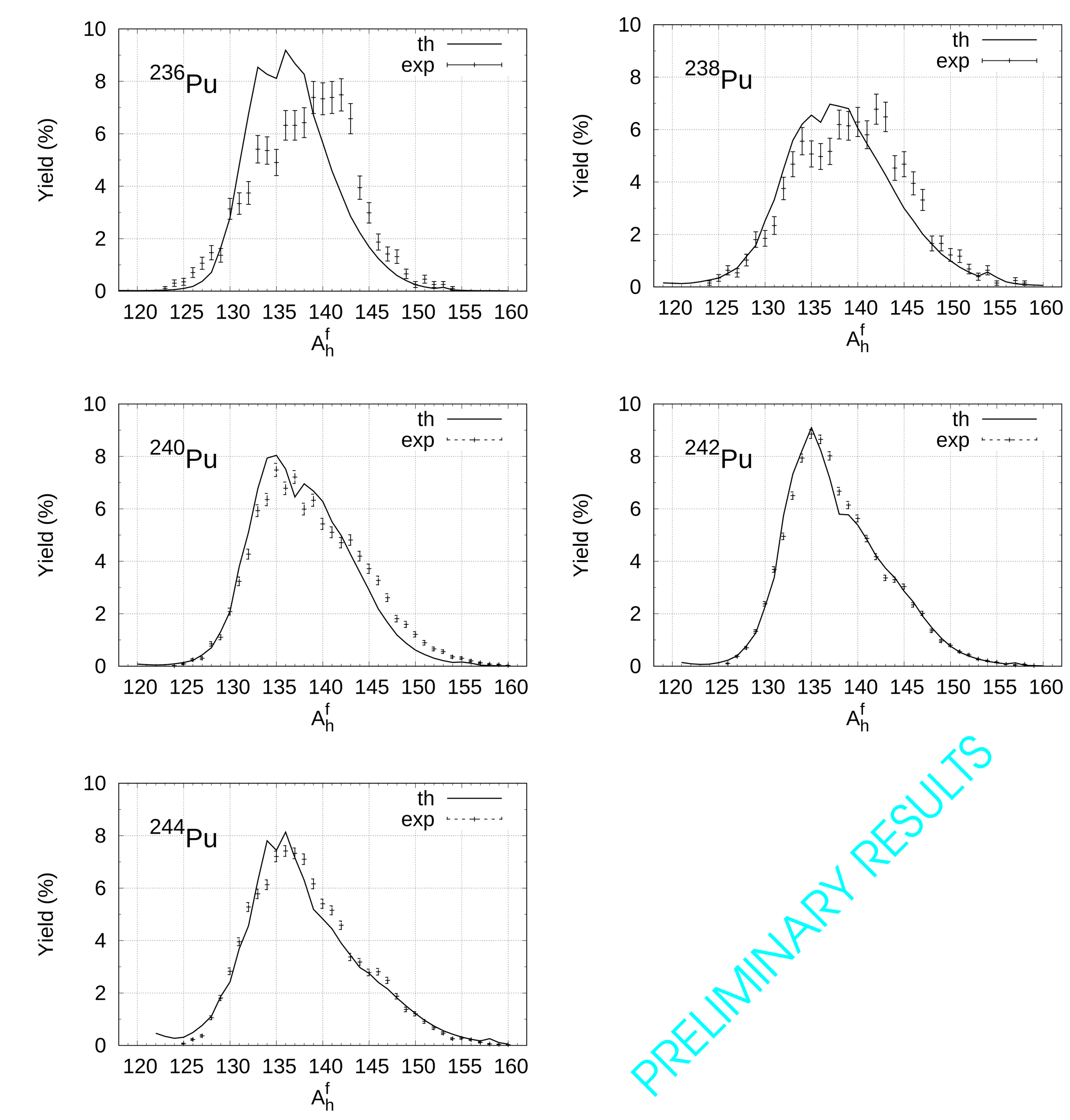

FIGURE 3: Experimental fission fragment mass yield for $^{236-244}$Pu isotopes [12] compared with preliminary estimates done with the Wigner function (14) for $E_0 \approx 2$ MeV.

Summary

It was shown in Ref. [6] that the three-dimensional quantum mechanical model which couples the fission, neck and mass asymmetry modes is able to reproduce the main features of the fragment mass distribution when the neck dependent fission probability is taken into account. The distribution obtained in [6] for ^{238}U reproduces nicely the structure of the distribution observed in the experiment. Preliminary results for the Plutonium isotopes also show that our model will give the fission fragment mass yield close to the measured distributions. Further calculations are in progress.

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