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FISSION FRAGMENTS MASS DISTRIBUTION OF ^{236}U*

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The fission fragments mass-yield is obtained by an approximate solution of the eigenproblem of the two-dimensional collective Hamiltonian corresponding to the fission and mass asymmetry modes. The potential energy surface was calculated by the macroscopic–microscopic method using the liquid drop model for the macroscopic part. The microscopic corrections were obtained using the Woods–Saxon single particle levels. The modified Cassini ovals shape parametrization in four dimensions was used to evaluate the potential energy surface. The mass tensor is taken within the cranking-type approximation.

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1. Introduction

A proper reproduction of the fission fragments mass distribution is one of the most important tests of any theoretical model describing the nuclear fission process. In the present paper, we are going to obtain such a distribution by an approximate solution of the eigenproblem of the two-dimensional collective Hamiltonian corresponding to the fission and mass asymmetry modes. The nonadiabatic and dissipative effects in low-energy fission were taken into account in a similar way as in Refs. [1, 2]. The potential energy surface (PES) was obtained by the macroscopic–microscopic method using the liquid drop model for the macroscopic part of the energy, while the microscopic shell and pairing corrections were calculated using the Woods–Saxon (WS) single particle levels [3]. The shape of the fissioning nucleus

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was described by the four-dimensional modified Cassini ovals (MCO) [3, 4]. It was shown in Ref. [5] that the MCO describe very well the optimal in energy shapes of nuclei even those close to the scission configuration. The mass tensor is taken within the cranking-type approximation (confer *e.g.* Sec. 5.1.1 of Ref. [6]).

Within the Born–Oppenheimer approximation (BOA), the wave function of the fissioning nucleus can be written in a form of product of the wave function $U(q)$ describing the motion towards fission and the function $W(\alpha, x; q)$ which depends on all others coordinates

$$\Psi(q, \alpha, x) = U(q)\, W(\alpha, x; q)\,. \tag{1}$$

Here, q is the fission coordinate, *e.g.* the distance between mass centres of the fragments, while α stays for other collective coordinates (*e.g.* mass asymmetry) and x represents the single-particle coordinates. One assumes in the BOA that the motion towards fission is slower than in the other degrees of freedom. In the adiabatic approximation, we assume that the function $W(\alpha, x; q)$ belongs to the lowest eigenvalue of the partial (internal) Hamiltonian $H_{\text{int}}(\alpha, x; q)$ defined for each value of q in the α, x coordinates.

The next step towards the inclusion of the finite fission velocity effects, called in the following nonadiabatic effects, will consist of expanding the wave function of the fissioning nucleus in a basis which describes excited states in the α-, x-, q-space

$$\psi(q, \alpha, x) = \sum_{m,k} C_{mk} U_{mk}(q) W_m(\alpha, x; q)\,. \tag{2}$$

Here, $W_m(\alpha, x; q)$ is an eigenfunction of the internal Hamiltonian which depends parametrically on q

$$\hat{H}_{\text{int}}(\alpha, x; q) W_m(\alpha, x; q) = \varepsilon_m(q) W_m(\alpha, x; q)\,. \tag{3}$$

The fission wave function $U(q)_{mk}$ depends on the quantum numbers m of the internal state via the energy $\varepsilon_m(q)$ and on the quantum numbers k which characterize the fission mode (energy, angular momentum *etc.*).

The dissipative effects which appear also in the low-energy fission process are simulated by adding an imaginary part to the collective potential [2].

The paper is organized in the following way. First, we present shortly the details of the theoretical model, then we show the collective potential energy surface evaluated in the macroscopic–microscopic model for ^{236}U and the components of the mass tensor calculated in the cranking approximation. The calculated fission fragments mass distribution is compared with the experimental data in the next section. Conclusions and plans of further calculations are presented in the summary.

2. Model

We use in the following two collective coordinates only:

$$q_1 = q = R_{12}/R_0 \qquad \text{and} \qquad q_2 = \alpha(V_1 - V_2)/(V_1 + V_2)\,, \tag{4}$$

where R_{12}/R_0 is the distance between the nascent fragments in units of the radius of the spherical nucleus, while V_1 and V_2 are the volumes of the fragments. Of course, one can introduce more collective coordinates, *e.g.* the one connected with the neck formation.

With these coordinates, the classical energy of the system becomes

$$H_a = \frac{1}{2}\sum_{i,j} M_{ij}\dot{q}^i\dot{q}^j + V\left(\{q^i\}\right)\,, \tag{5}$$

where M_{ij} and $V(\{q^i\})$ denote the mass tensor and the potential energy, respectively.

The quantized form of this Hamiltonian is the following:

$$\widehat{H} = -\frac{\hbar^2}{2}\sum_{i,j} |M|^{-1/2}\frac{\partial}{\partial q^i}|M|^{-1/2}M^{ij}\frac{\partial}{\partial q^j} + V\left(\{q^i\}\right)\,, \tag{6}$$

where $|M| = \det(M_{ij})$ and $M_{ij}M^{jk} = \delta_i^k$.

In the two-dimensional space $(q,\,\alpha)$ the mass tensor is

$$M_{ij} = \begin{pmatrix} M_{qq} & M_{q\alpha} \\ M_{\alpha q} & M_{\alpha\alpha} \end{pmatrix}. \tag{7}$$

We chose a coordinate system $q_i = (q,\alpha)$ in such a way that the mass tensor is diagonal, *i.e.* $M_{q\alpha} = M_{\alpha q} = 0$. This condition can always be fulfilled in the two-dimensional space. For simplicity, we denote in the following the diagonal elements of the mass tensor as:

$$M_q \equiv M_{qq}(q,\alpha)\,, \qquad M_\alpha \equiv M_{\alpha\alpha}(q,\alpha)\,. \tag{8}$$

According to the above, to describe the fission process, one has then to solve the eigenproblem with the collective Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\frac{1}{\sqrt{M_q M_\alpha}}\left[\frac{\partial}{\partial q}\sqrt{\frac{M_\alpha}{M_q}}\frac{\partial}{\partial q} + \frac{\partial}{\partial \alpha}\sqrt{\frac{M_q}{M_\alpha}}\frac{\partial}{\partial \alpha}\right] + V\,. \tag{9}$$

Note that the scalar product of the eigenfunctions φ_i of the Hamiltonian $\widehat{H}$

$$(\varphi_i|\varphi_j) = \int\!\!\int \varphi_i^*(q,\alpha)\varphi_j(q,\alpha)D(q,\alpha)dqd\alpha \tag{10}$$

is defined with the metric

$$D(q,\alpha) = \sqrt{M_q(q,\alpha) M_\alpha(q,\alpha)}\,. \tag{11}$$

It is useful to work with the wave functions $\tilde{\varphi}_i$ which would be orthogonal without a complicated metric

$$(\tilde{\varphi}_1|\tilde{\varphi}_2) = \int\int \tilde{\varphi}_1^*(q,\alpha)\tilde{\varphi}_2(q,\alpha)dqd\alpha\,. \tag{12}$$

To this aim, we perform now an unitary transformation of the Hamiltonian $\widehat{H}$ and its eigenfunctions $\varphi(q,\alpha)$ with the help of the function $\sqrt{D(q,\alpha)}$

$$\begin{aligned} \tilde{\varphi}(q,\alpha) &= \sqrt{D(q,\alpha)}\,\varphi(q,\alpha)\,, \\ \tilde{H}(q,\alpha) &= \sqrt{D(q,\alpha)}\,\widehat{H}(q,\alpha)\sqrt{D(q,\alpha)}^{\,-1}\,. \end{aligned} \tag{13}$$

Then, the Hamiltonian takes the form

$$\tilde{H} = -\frac{\hbar^2}{2}\left[\frac{\partial}{\partial q}\frac{1}{M_q}\frac{\partial}{\partial q} + \frac{\partial}{\partial \alpha}\frac{1}{M_\alpha}\frac{\partial}{\partial \alpha}\right] + V(q,\alpha) + V_G(q,\alpha)\,. \tag{14}$$

Neglecting the small scalar term $V_G(q,\alpha)$, we split up $\tilde{H}$ into the kinetic energy operator $\tilde{T}_q$ responsible for the motion towards fission and the adiabatic Hamiltonian in perpendicular to the fission mode direction

$$H_\alpha^{\rm ad}(\alpha;q) = -\frac{\hbar^2}{2}\frac{\partial}{\partial\alpha}\frac{1}{M_\alpha(\alpha;q)}\frac{\partial}{\partial\alpha} + V(\alpha;q)\,. \tag{15}$$

The Hamiltonian $H_\alpha^{\rm ad}$ has the eigenfunctions W_m

$$H_\alpha^{\rm ad}(\alpha;q)W_m(\alpha;q) = \varepsilon_m(q)W_m(\alpha;q)\,, \qquad \text{where} \qquad m = 1,2,\ldots \tag{16}$$

In order to define the adiabatic part of $\tilde{T}_q$, we introduce the average mass

$$\overline{M}_q(q) = \int W_1^*(\alpha;q)M_q(q,\alpha)W_1(\alpha;q)/|W_1(\alpha;q)|^2 d\alpha\,. \tag{17}$$

Then, $T_q^{\rm ad}$ is defined by

$$T_q^{\rm ad}(q) = -\frac{\hbar^2}{2}\frac{\partial}{\partial q}\frac{1}{\overline{M}_q(q)}\frac{\partial}{\partial q}\,. \tag{18}$$

The eigenfunctions of the total adiabatic Hamiltonian

$$H^{\rm ad}(q,\alpha) = T_q^{\rm ad}(q) + H_{\alpha;q}^{\rm ad} \tag{19}$$

can be written as

$$\varphi^{\rm ad}_{nE}(q,\alpha) = U_{nE}(q) W_n(\alpha, x; q)\,. \tag{20}$$

The adiabatic Schrödinger equation is

$$\left(T^{\rm ad}_q + H^{\rm ad}_\alpha\right)\, U_{nE}(q) W_n(\alpha, x; q) = E\, U_{nE}(q) W_n(\alpha, x; q)\,, \tag{21}$$

which with Eq. (16) yields the following equation for the fission mode wave function:

$$\left(T^{\rm ad}_q + \varepsilon_n(q)\right)\, U_{nE}(q) = E\, U_{nE}(q)\,. \tag{22}$$

The energies $\varepsilon_n(q)$ define the fission potential when the fission takes place by the $n^{\rm th}$ channel W_n, where $n = 1, 2, 3, \ldots$ The approximate solution of the above eigenproblem can be obtained using the WKB formalism.

The wave function Ψ_E we are looking for contains in addition to the adiabatic wave function $\phi^{\rm ad}_{1E}$ other contributions $\phi^{\rm ad}_{nE}$

$$\Psi_E(q,\alpha) = \varphi^{\rm ad}_{1E}(q,\alpha) + \sum_{n>1}^{M} \int dE'\, C_n\left(E, E'\right)\, \varphi^{\rm ad}_{nE'}(q,\alpha)\,. \tag{23}$$

We make the following ansatz for the coefficients $C_n(E, E')$:

$$C_n\left(E, E'\right) = \sum_{k=1}^{k_{\rm max}} a_{nk}\, h_k\left(\frac{E-E'}{\Delta E}\right) \exp\left[-\left(\frac{E-E'}{\Delta E}\right)^2\right]\,, \tag{24}$$

which allows the system to go off shell in the fission energy up to $|E-E'| \simeq \Delta E$. Here, h_k is the Hermite polynomial of the order of k.

The coefficients a_{nk} are determined from the requirement

$$\frac{\partial}{\partial a_{nk}}\left[\int \Psi^*_E (H-E)^2 \Psi_E\, N^2(q)\, dq d\alpha\right] = 0\,, \tag{25}$$

where $N^2(q) = |U_{1E}(q)|^{-2}$ is the normalization factor.

The above variational procedure leads to a system of linear equations for the coefficients a_{nk} [2]. The width ΔE is determined from the requirement that the norm of $(H-E)\Psi_E(q,\alpha)$ should be as small as possible.

Energy dissipation on the classical part of the fission path from the turning $q_{\rm turn}$ point to the scission point $q_{\rm sci}$ is included by adding an imaginary part to the fission potential which was chosen here of the simplest linear form

$$V_{\rm imag} = \begin{cases} 0 & \text{for} \quad q < q_{\rm turn}\,, \\ c(E-V) & \text{for} \quad q_{\rm turn} \le q \le q_{\rm sci}\,, \end{cases} \tag{26}$$

where c is an arbitrary coefficient and $q_{\rm turn}$ corresponds to the point in which $V = E$. More elaborated expression for $V_{\rm imag}$ was derived in Ref. [2].

3. Results

The potential energy surface was evaluated for ^{236}U at zero temperature within the macroscopic–microscopic model in which the macroscopic part of the energy was obtained using the liquid drop formula and the microscopic shell and pairing corrections were calculated using the Woods–Saxon single-particle potential. All parameters of the calculation are described in Ref. [4]. The inertia tensor was evaluated using the cranking approximation. The calculations were performed in a 4-dimensional space of deformation parameters $\alpha_0, \alpha_1, \alpha_4, \alpha_6$ [4]. For each value of α_4 and α_6, the potential energy was transformed from α_0, α_1 to R_{12}, α coordinates defined in Eq. (4). The energy of each grid point in the (R_{12}, α) space was minimized then with respect to α_4 and α_6. An example of the so-minimized PES and the components of the inertia tensor for ^{236}U is shown in Fig. 1. These quantities were used to construct the collective Hamiltonian (9). For simplicity, we have neglected here the nondiagonal component of the mass tensor as $|M_{q\alpha}| \ll M_{\alpha\alpha}$. All parameters of the collective model are the same as in Ref. [2].

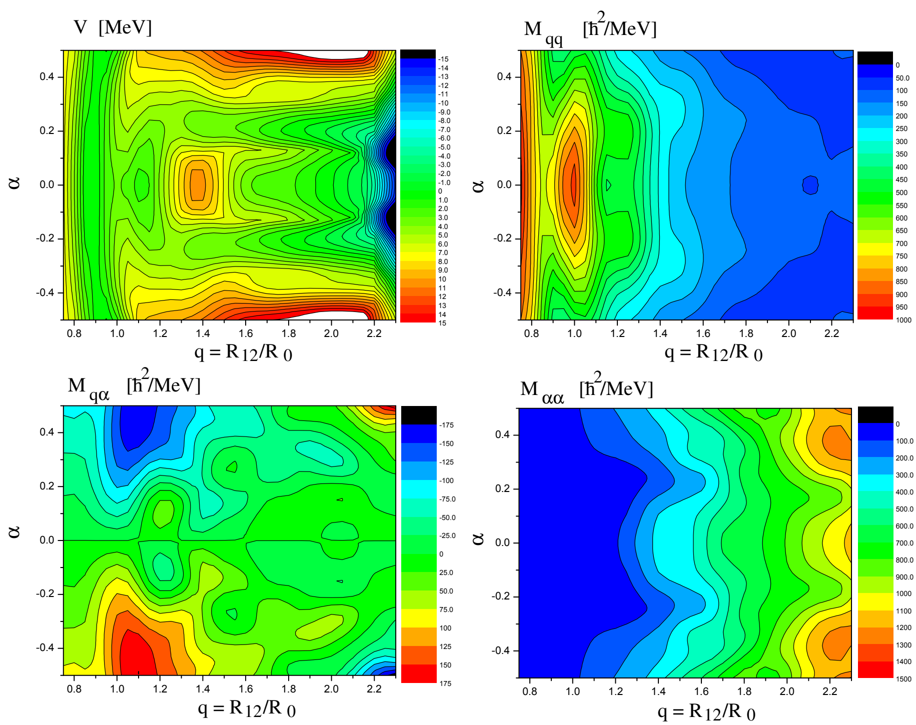

Fig. 1. PES and cranking inertia tensor for ^{236}U as functions of the elongation (R_{12}/R_0) of nucleus and the mass asymmetry.

The probability distributions for the masses of the fission fragments are obtained from the total wave function (23) for $q \simeq q_{\rm sc}$

$$|P_E(\alpha)|^2 = |\Psi_E(q = q_{\rm sc}, \alpha)|^2 \,. \tag{27}$$

The evaluated fission fragment mass distributions are presented in Fig. 2 for different elongation (R_{12}/R_0) of the fissioning nucleus. The mass-yield obtained without dissipation is presented in the left panel, while the result obtained with the dissipation ($V_{\rm imag} \neq 0$) are shown in the right panel. It is seen in the both figures that a sudden change of the predicted mass

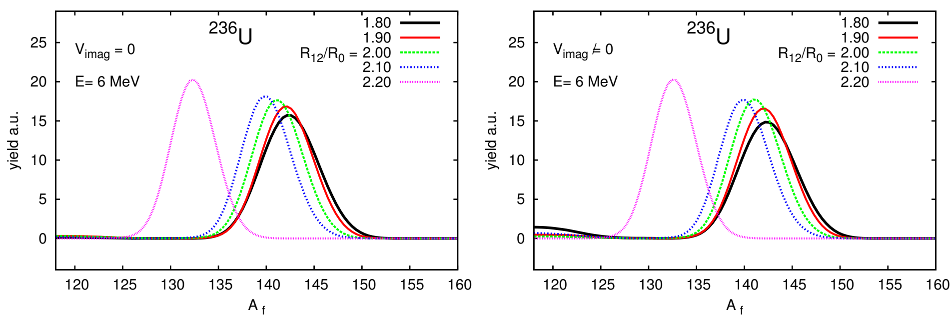

Fig. 2. Fission fragment mass distribution of ^{236}U obtained without (l.h.s.) and with $V_{\rm imag}$ (r.h.s.) as function of the mass of the heavier fragment $A_{\rm f}$. Different curves correspond to the various elongations of the fissioning nucleus.

yield takes place when the elongation varies from 2.1 to 2.2. This effect appears due to the minimization procedure when the information on higher order deformations is partly lost. This minimization makes possible to "see" only one fission valley. Hence, the PES of Fig. 2 demonstrates that the

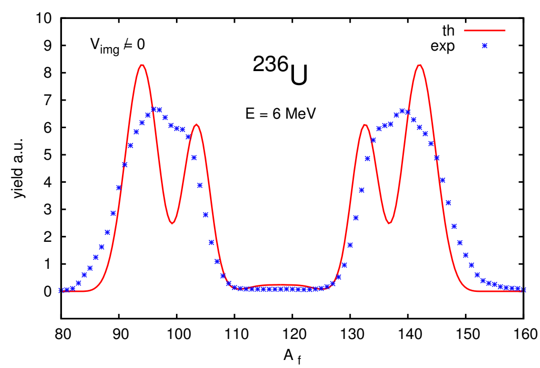

Fig. 3. Weighted sum of the mass yields corresponding to the $A_{\rm f} = 140$ and $A_{\rm f} = 132$ valleys mixture compared with the data [7].

minimization (which follows always the minimum valley) leads to a jump from the $A = 140$ mode at shorter R_{12} to the $A = 132$ mode at larger R_{12}. Including the neck degree of freedom will permit to preserve both valleys all along the R_{12} axis, and thus the proposed approach would populate them according the their depth and inertia features. A mixture of the theoretical mass yields corresponding to the two above valleys is compared in Fig. 3 with the data [7]. The yield for $R_{12}/R_0 = 1.9$ is taken in Fig. 3 with the weight 5/8 and that for 2.2 with 3/8.

4. Conclusions

We have shown that the two-dimensional quantum mechanical model which couples the fission and mass asymmetry modes is able to describe the main features of the mass distribution of the fragments. The extended Cassini ovals deformation parameters and the macroscopic–microscopic model (E_{LD} plus the WS s.p. potential) lifers for ^{236}U a PES with the asymmetric fission valley corresponding to $A_{\mathrm{f}} \approx 140$. The nonadiabatic effects (beyond the Born–Oppenheimer app.) make the distributions slightly wider than the sole adiabatic ones. The energy dissipation (due to the presence of a imaginary part in the fission potential) enlarge further the distribution towards larger mass asymmetry. The neck degree of freedom should be added to the model as the third collective coordinate in order to obtain the proper scission configurations.

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