To fission or not to fission

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The fission-fragments mass-yield of $^{236}$U is obtained by an approximate solution of the eigenvalue problem of the collective Hamiltonian that describes the dynamics of the fission process whose degrees of freedom are: the fission (elongation), the neck and the mass-asymmetry mode. The macroscopic-microscopic method is used to evaluate the potential energy surface. The macroscopic energy part is calculated using the liquid drop model and the microscopic corrections are obtained using the Woods-Saxon single-particle levels. The four dimensional modified Cassini ovals shape parametrization is used to describe the shape of the fissioning nucleus. The mass tensor is taken within the cranking-type approximation. The final fragment mass distribution is obtained by weighting the adiabatic density distribution in the collective space with the neck-dependent fission probability. The neck degree of freedom is found to play a significant role in determining that final fragment mass distribution.

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I. INTRODUCTION

A very stringent test of any theoretical model which describes the nuclear fission process should be a proper reproduction of the fission fragments mass distribution. The goal of the present paper is to obtain such a distribution by an approximate solution of the eigenvalue problem of the 3-dimensional collective Hamiltonian with degrees of freedom corresponding to elongation, neck formation and mass asymmetry of the nuclear shape. The present model is similar to the 2-dimensional one of Refs. [1,2] but the non-adiabatic and dissipative effects are not taken here into account since their effect is rather small for low-temperature fission. The potential energy surface (PES) is obtained in the present work using the microscopic-microscopic method with the liquid drop model for the macroscopic part of the energy while the microscopic shell and pairing corrections are calculated using the Woods-Saxon (WS) single-particle levels [3]. The shape of the fissioning nucleus is described by the four dimensional modified Cassini ovals (MCO) [3,4]. It was shown in Ref. [3] that the MCO describe very well the so-called optimal nuclear shapes obtained through a variational description [6], 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. [1]). The Born-Oppenheimer approximation (BOA) is used to describe the coupling of the fission mode with the neck and mass asymmetry degrees of freedom. It will be shown that, in order to obtain a fission-fragment mass distribution in agreement with the experimental data, that fission probability should depend on the neck size.

The paper is organized in the following way. First we shortly present the details of our 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. The calculated fission fragments mass distribution is compared with the experimental data in the next section. Conclusions and possible extensions and applications of our model are presented in Summary.

II. COLLECTIVE HAMILTONIAN

A. Shape parameterization

We define the shape of fissioning nucleus by the parameterization developed in [3]. In this parameterization some cylindrical co-ordinates {$\varpi, \tau$} are related to the lemniscate co-ordinates system {$R, x$} by the equations

$$p = \frac{1}{\sqrt{2}} \sqrt{p(x) - R^2(2x^2 - 1) - s},$$

$$\tau = \frac{\text{sign}(x)}{\sqrt{2}} \sqrt{p(x) + R^2(2x^2 - 1) + s},$$

$$p^2(x) \equiv R^4 + 2sR^2(2x^2 - 1) + s^2,$$

$$0 \leq R \leq \infty, -1 \leq x \leq 1.$$  

The co-ordinate surfaces of the lemniscate system $R(x) = R_0$ are the Cassini ovals (see the bottom of Fig. 1) with $s \equiv \varepsilon R_0^2$, where $s$ is the squared distance between the focus of Cassinian ovals and the origin of coordinates.

The deviation of the nuclear surface from Cassini ovals is defined by expansion of $R(x)$ in series in Legendre poly-

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The deformation parameters α describe the neck degree of freedom when \( R_{12} \) is kept constant (see Ref. [2]).

With these coordinates the classical energy of the system becomes

\[
H_{cl} = \frac{1}{2} \sum_{i,j} M_{ij} \dot{q}_i \dot{q}_j + V(\{q_i\}),
\]

where \( M_{ij} \) and \( V(\{q_i\}) \) denote the inertia tensor and the potential energy, respectively.

The quantized form of this Hamiltonian is the following:

\[
\hat{H} = -\frac{\hbar^2}{2} \sum_{i,j} |M|^{-1/2} \frac{\partial}{\partial q_i} |M|^{-1/2} M^{ij} \frac{\partial}{\partial q_j} + V(\{q_i\}),
\]

where \(|M| = \det(M_{ij})\) and \( M_{ij} M^{jk} = \delta_{ik} \).

The eigenproblem of this Hamiltonian will be solved here in the Born-Oppenheimer approximation in which one assumes that the motion towards fission is much slower than the one in the two other collective coordinates. In such an approximation the Hamiltonian could be written as follows:

\[
\hat{H}(R_{12}, a, \alpha_4) \approx \hat{T}_{fs}(R_{12}) + \hat{H}_{perp}(a, \alpha_4; R_{12}).
\]

Here \( \hat{T}_{fs} \) is the fission mode kinetic energy operator

\[
\hat{T}_{fs}(R_{12}) = -\frac{\hbar^2}{2} \frac{\partial}{\partial R_{12}} \mathcal{M}^{-1}(R_{12}) \frac{\partial}{\partial R_{12}},
\]

where \( \mathcal{M}(R_{12}) \) is the average inertia related to the fission mode and \( \hat{H}_{perp} \) is the collective Hamiltonian related to the neck and mass asymmetry coordinates. The eigenfunction of Hamiltonian [3] can be written as a product:

\[
\Psi_{nE}(R_{12}, a, \alpha_4) = u_{nE}(R_{12}) \varphi_n(a, \alpha_4; R_{12}),
\]

where \( \varphi_n \) are the eigenfunctions of \( \hat{H}_{perp} \):

\[
\hat{H}_{perp} \varphi_n(a, \alpha_4; R_{12}) = e_n(R_{12}) \varphi_n(a, \alpha_4; R_{12}),
\]

and they are evaluated for each mesh-point value in the \( R_{12} \) direction. Using the above relations one can rewrite the eigenequation of the Hamiltonian [3] in the following form:

\[
\left( \hat{T}_{fs} + e_n(R_{12}) \right) u_{nE}(R_{12}) = E u_{nE}(R_{12}).
\]

The approximate solution of the above eigenvalue problem can be obtained using the WKB formalism. The energies \( e_n(R_{12}) \) in Eq. [12] define the fission potential for different channels, what is important when one describes the nonadiabatic fission process in the coupled channels approach [2]. In the following we shall take only the lowest energy channel, what corresponds to the adiabatic approximation. Within this approximation the wave function of the fissioning nucleus is written in the form of a product of the wave function \( u_{nE}(R_{12}) \) describing the motion towards fission and the function \( \varphi_n(a, \alpha_4; R_{12}) \) which corresponds to the lowest eigenenergy \( e_0 \) of the Hamiltonian [11]. The probability of finding of a nucleus, for a...
given value of $R_{12}$, in the given $(a, \alpha_4)$ point is equal to $|\varphi_0(a, \alpha_4; R_{12})|^2$.

In Refs. [1,2] is shown how to go beyond the BOA and include nonadiabatic and dissipative effects, but in the following we are going to omit such effects, which are expected to be small at low temperatures and limit our discussion to the effect of the neck degree of freedom on the fission-fragment mass distribution.

### III. NUMERICAL RESULTS

The potential energy surface is evaluated for $^{236}\text{U}$ at zero temperature within the macroscopic-microscopic model in which the macroscopic part of the energy is obtained using the liquid drop formula and the microscopic shell and pairing corrections are calculated using the Woods-Saxon single-particle potential. All parameters of the calculation are described in Ref. [4]. The potential energy was calculated in 4-dimensional space of deformation parameters $\alpha, \alpha_1, \alpha_4, \alpha_6$ and minimized then with respect to $\alpha_6$.

The mass parameter $M_{ij}(q)$ for the fission process is commonly calculated by the Inglis formula

$$M_{ij}(q) = 2\hbar^2 \sum_m \frac{\langle 0 | \partial q | m \rangle \langle m | \partial q | 0 \rangle}{E_m - E_0},$$

where $|0\rangle$ and $|m\rangle$ denote the ground and an excited state of the system.

In the case that the ground and the excited states of the system are described by the BCS approximation, the $M_{ij}(q)$ is given by [9],

$$M_{ij} = 2\hbar^2 \sum_{\mu\nu} \frac{\langle \mu | \partial q | \nu \rangle \langle \nu | \partial q | \mu \rangle}{(E_{\mu} + E_{\nu})^3} \eta_{\mu\nu}^2 + P_{ij},$$

(14)

where the term $P_{ij}$ stands for the contribution due to the change of occupation numbers, when the deformation varies. The $E_{\mu}$, $u_\mu$, and $v_\mu$ in (14) are the quasi-particle energies and coefficients of the Bogolyubov-Valatin transformation correspondingly, and $\eta_{\mu\nu} = u_\mu v_\nu + u_\nu v_\mu$.

Unfortunately, the expression (14) has the very unpleasant feature that it does not turn into the mass parameter of a system of independent particles when the pairing vanishes, $\Delta \to 0$. More precisely, the non diagonal sum over single-particle states in (14) does turn into the mass parameters of the system of independent particles when $\Delta \to 0$, but, even worse, the diagonal sum goes to infinity in that limit (it is proportional to $1/\Delta^2$, as demonstrated in [8]). Thus, at some points in the deformation space, where the density of single-particle states is very low, the mass parameter (14) becomes unreasonably large. The same happens in excited systems, when the temperature is close to its critical value $T_{crit}$ at which the pairing gap disappears.

One should also keep in mind that the diagonal contribution to the sum in (14) comes from the matrix elements between the ground state and the pair excited states that correspond to the particle number, different from that of the ground state. In a particle number conserving theory such contribution could not appear.

In order to avoid the problems related to the diagonal contribution to (14) we have omitted in (14) the diagonal matrix elements $\langle \mu | \partial q | \nu \rangle$ and taken into account only the non-diagonal part of (14).

$$M_{ij} = 2\hbar^2 \sum_{\mu \neq \nu} \frac{\langle \mu | \partial q | \nu \rangle \langle \nu | \partial q | \mu \rangle}{(E_{\mu} + E_{\nu})^3} \eta_{\mu\nu}^2.$$  

(15)

The inertia tensor (15) is evaluated in the 3-dimensional space of deformation parameters $\alpha, \alpha_1, \alpha_4$. For each value of $\alpha_4$ and the potential energy and the components of mass tensor were transformed from $\alpha, \alpha_1$ to $R_{12}$, a coordinates defined in Eq. [4]. The potential energy surface (PES) related to the spherical liquid drop energy (upper row) and the $M_{R_{12}R_{12}}$ component of the inertia tensor (middle row) as well as the neck radius $\kappa = r_{neck}/R_0$ (lower row) are plotted in Fig. 2 on the $(A_t, \alpha_4)$ plane for three different values of the relative distances of the center of the fragments $R_{12}$. Here $A_t$ is the atomic mass of fission fragment.

In the following we would like to describe the way in which one has to obtain the fission fragment mass yield after solving the quantum mechanical problem of the collective Hamiltonian which describes the fission process in the three dimensional space (3D) composed of the following deformation parameters:

- $R_{12} =$ distance between the mass center of the fission fragments,
- $a =$ $[A_t(1) - A_t(2)]/[A_t(1) + A_t(2)]$ $-$ the mass asymmetry parameter, where $A_t(1)$ and $A_t(2)$ are the mass numbers of the fission fragments,
- $\alpha_4 =$ hexadecapole correction to the Cassini ovals [3].

First one has to prepare a set of the 2D mass distributions

$$|\Psi(a, \alpha_4; R_{12})|^2 = |\varphi_0(a, \alpha_4; R_{12})|^2$$  

(16)

on the plane $(a, \alpha_4)$ by solving eigenproblem of a corresponding 2D collective Hamiltonian for fixed elongations $R_{12}$ [8]. One has to bear in mind that it is very unlikely, that fission occurs at some fixed $R_{12}$ or when the system reaches the scission line/surface. The problem is much more complicated and one has to involve into consideration the size of the neck.

Looking at the integrated over $\alpha_4$ probability distributions for $^{236}\text{U}$ presented in the top part of Fig. 3

$$w(a, R_{12}) = \int |\Psi(a, \alpha_4; R_{12})|^2 d\alpha_4,$$  

(17)

one can not see any qualitative change with respect to the results which we have published in Ref. [2] for the calculation made in the $(R_{12}, a)$ plane. Both distributions, i.e. the one corresponding to $A_t(1) = 140$ for smaller
FIG. 2: (Color online) Macroscopic-microscopic PES (upper row) and the relative distance component $M_{R_{12}R_{12}}$ of the inertia tensor (middle row) and the neck radius $\kappa = r_{\text{neck}}/R_0$ (lower row) on the $(A_f, \alpha_4)$ plane for different values of the elongation $R_{12}$. 

$R_{12}$ and the one for $A_f(1) = 132$ at $R_{12}$ close to the scission line are only slightly broader. So, the problem to reproduce the experimental distribution of fission fragments, seen in the 2D space [2], remains also in the 3D space. The only solution is to assume that fission occurs with a certain probability before (or after) reaching the critical elongation $R_{12}^{\text{crit}}$. 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. Of course this is not a Hamlet dilemma, where there is only the choice between yes or no. We are rather faced here with a statistical problem and the answer yes is given with a certain probability which one then will have to take into account in the distribution probability (16) in the phase space.

Following such an assumption a part of the events (read trajectories in the Langevin approach, or distributions in our quantum mechanical model) disappears from the phase-space and leads to a kind of weighting of the mass distribution corresponding to the different elongations $R_{12}$. To do this one has to evaluate the neck radius in the whole 3D space. The neck radius parameter $\kappa = r_{\text{neck}}/R_0$ is plotted in the lower row of Fig. 2 on the $(A_f, \alpha_4)$ plane for three different values of the elongation parameter $R_{12}$. The slight wiggles in Fig. 2 are caused by the approximate minimization with respect to the $\alpha_6$ deformation parameter. It is seen that on average the neck radius decreases with growing $R_{12}$. For a constant $R_{12}$ the neck radius varies strongly with $\alpha_4$ and $A_f$. One commonly agrees that fission takes place when the neck radius becomes of the order of the size of a nucleon. This is the case for $\kappa \approx 0.2$, which is realized at $R_{12}/R_0 = 2.0$ for $\alpha_4 = -0.18$; $R_{12}/R_0 = 2.25$ for $\alpha_4 = 0$, and $R_{12}/R_0 > 2.5$ for $\alpha_4 = 0.18$ and the asymmetry parameter $\alpha \approx 0.2$. From the optimal shape approach [8] one knows that the scission shape corresponds to $r_{\text{neck}} \approx 0.3R_0$ and $R_{12}^{\text{crit}} \approx 2.3R_0$. In the case of the Cassini parametrization used in the present paper the $r_{\text{neck}}$ can be somewhat smaller.

One could try to parametrize the neck-rupture proba-
probability \( P \) in the following form:

\[
P(a, \alpha_4, R_{12}) = \frac{k_0}{k} P_{\text{neck}}(\kappa) ,
\]

where \( k \) is the momentum in the direction towards fission (or simply the velocity along the elongation coordinate \( R_{12} \)), while \( \kappa = \kappa(a, \alpha_4, R_{12}) \) 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 when one will normalize it. The geometry dependent part of the neck breaking probability is taken in the form of a Fermi function:

\[
P_{\text{neck}}(\kappa) = \left( 1 + e^{-\frac{\kappa - \kappa_0}{d}} \right)^{-1} .
\]

The parameters \( \kappa_0 \) and \( d \) have to be fixed by comparing the theoretical fission fragment mass distributions with the experimental ones. Our goal is to fix these parameters in a kind of universal way, independent of the specific fission reaction that one wants to investigate. The present investigation has to be treated only as a first attempt in this direction.

The momentum \( k \) which appears in the denominator of Eq. (18) has to ensure that the probability depends on time in which one crosses the subsequent intervals in \( R_{12} \) coordinates: \( \Delta t = \Delta R_{12}/v(R_{12}) \), where \( v(R_{12}) = \hbar k/M(R_{12}) \) is the velocity towards fission. The value of \( k \) depends on the difference \( E - V(R_{12}) \) and on the part of the collective energy which is converted into heat \( Q \):

\[
\frac{\hbar^2 k^2}{2M(R_{12})} = E_{\text{kin}} = E - Q - V(R_{12}) .
\]

In the quantum mechanical picture the heat \( Q \) can be replaced by the imaginary part of the collective potential \( \mathcal{V} \). In the Langevin picture the method should be almost the same but one has also to work at least in the 3D space. In our present calculations we have put \( Q = 0 \), i.e., we assumed a "complete acceleration" scenario: no dissipation takes place, which is reasonable since at low excitation energies the friction force is very week.

The \( \mathcal{M} \) in (20) is the cranking inertia relative to the \( R_{12} \) deformation parameter. In principle, we used the definition of cranking inertia, but for the reasons explained above the contributions from the diagonal matrix elements were removed.

The fission probability \( w \) at a given \( R_{12} \) and \( a \) will be given by the integral:

\[
w(a, R_{12}) = \int |\Psi(a, \alpha_4; R_{12})|^2 P(a, \alpha_4, R_{12}) d\alpha_4 . \tag{21}
\]

The dependence of the fission probability (21) on the mass asymmetry is shown in the bottom part of Fig. 3 for a few values of \( R_{12} \). One observes that due to the Fermi function in (19) the contribution of larger \( R_{12} \) (smaller necks) is enhanced and contributions from smaller \( R_{12} \) are suppressed.

From the maps of the potential energy surface shown in the top part of Fig. 2 one observes that for \( R_{12} \leq 2.1 \) the neck parameter is \( \alpha_4 = -0.05 \) while for \( R_{12} \geq 2.2 \) the minimum at the PES is at \( \alpha_4 = -0.15 \). This means that a large part of the distribution probability \( |\Psi(a, \alpha_4; R_{12})|^2 \) will undergo fission also at smaller elongations and one has to subtract this part from the phase-space, i.e. to diminish the initial distribution by subtracting the events which have already fissioned. The final (measured) mass distribution of the fission fragments will be the sum of those subtracted events.

Such an approach means that the fission process should be spread over some region of \( R_{12} \) and that for given \( R_{12} \) at fixed mass asymmetry one has to take into account the probability to fission at previous \( R_{12} \) points. I.e., one has to replace \( w(a, R_{12}) \) by

\[
w'(a, R_{12}) = w(a, R_{12}) \left( 1 - \frac{\int_{R_{12}' \leq R_{12}} w(a, R_{12}') dR_{12}'}{\int w(a, R_{12}') dR_{12}'} \right) . \tag{22}
\]

The effect of the replacement (22) is demonstrated in Fig. 3. It is seen there that this replacement substantially reduces the magnitude of the fission probability at large \( R_{12} \).

The mass yield will be the sum of all partial yields at different \( R_{12} \):

\[
Y(a) = \frac{\int w'(a, R_{12}) dR_{12}}{\int w'(a, R_{12}) dR_{12} da} . \tag{23}
\]

As it is seen from (23) the scaling factor \( k_0 \) in the expression for \( P \), Eq. (18), has vanished and does not appear in...
the definition of the mass yield. Our model will thus only have two adjustable parameters, $\kappa_0$ and $d$, that appear in the neck-breaking probability $|W|$.)

A comparison of the measured [10] and here calculated fission fragment mass distributions is shown in Fig. 5 for the thermal neutron induced fission of $^{235}\text{U}$. One can see that the calculated mass distribution is very close to the experimental values. The double-peak structure, the position and the relative magnitude of the peaks are reproduced rather well.

IV. CONCLUSIONS

The extended Cassini ovals deformation parameters and the macroscopic-microscopic model ($E_{\text{LD}}$ plus the WS single-particle potential) yields for $^{236}\text{U}$ a PES with an asymmetric fission valley corresponding to $A_f \approx 140$ when the relative distance between the fragment mass centers is smaller than $R_{12} = 2.3R_0$. At larger elongations one observes a sudden jump of the maximum of the distribution to $A_f \approx 132$ what causes severe problems in a correct reproduction of the data.

We have shown that the three-dimensional quantum mechanical model which couples the fission, neck and mass asymmetry modes is able to describe the main features of the fragment mass distribution when the neck dependent fission probability is taken into account. The obtained mass distribution is slightly shifted, by approximately 2 mass units, towards symmetric fission as compared with the experimental mass yield, but reproduces nicely the structure of the distribution observed in the experiment. This shift could be partly due to a too large stiffness of the LD energy in the mass asymmetry degrees of freedom and/or to a lack of the nonadiabatic effects (beyond the Born-Oppenheimer app.) [2] which makes the distributions slightly wider than the sole adiabatic ones. Also the energy dissipation, not taken into account in the present investigation, could modify somewhat the theoretical distribution.

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