FISSION PATHS INFLUENCED BY PROTON AND NEUTRON MAGICITY

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The macroscopic-microscopic method is used to calculate penetrabilities for different fission channels around proton and neutron magic numbers from uranium and plutonium. The liquid drop part is obtained from the Yukawa-plus-exponential potential, whereas the single-particle energy levels are computed with the deformed two-center shell model. The shell correction part is obtained by the Strutinsky method, separately for protons and neutrons. Calculations are applied to the fission of U and Pu and penetrability values are presented for the most favoured channels. The dynamical part is approached through the multidimensional minimization of the action integral within the typical deformation space of nuclear binary processes.

Key words: Spontaneous fission, lifetimes, macroscopic-microscopic method, two-center shell model.

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1. INTRODUCTION

In fission experiments one has a weak distinction between different atomic numbers for the same mass asymmetry. The final charge splitting within a certain mass of the daughter and emitted fragment is the result of a balance between the macroscopic part of the energy and the influence of the quantum effects via the shell correction energy. In other words, for a given \( A_H \) and \( A_L \) emitted from the same parent nucleus, one has to find the most favourable charge asymmetry, or \( Z_H \) and \( Z_L \). The completely determined pair \((A_H, Z_H)\) and \((A_L, Z_L)\) are obtained as the two reaction partners emerged from the final minimization of the action integral of the process for a given parent nucleus. The study is equivalent to the treatment of isobaric nuclear systems by accounting for the charge density change during the overlapping part of the two emitted fragments. Isobaric systems have been treated for intermediate nuclei reactions, like for example in [1] for energies below the Bass barrier. Some other author’s approach have the hypothesis of unchanged charge density for nuclear fission [2].

This work is dedicated to the study of the favoured atomic numbers between fragments with the same mass for the fission of U and Pu parent nuclei. We will briefly present the specialized macroscopic-microscopic method in use for the total deformation energy calculation in section 2. Section 3 contains the shell correction method developed by Strutinsky and adapted to our special configuration. In section 4 the results of our calculation are presented, followed by conclusions.

2. THE MACROSCOPIC-MICROSCOPIC METHOD

2.1. NUCLEAR SHAPE PARAMETRIZATION

In these calculations the nuclear shapes are assumed to be two ellipsoids with \(a_1, b_1\) and \(a_2, b_2\), smoothly joined. Here we consider no neck. The two centers are in \((z_1,0)\) and \((z_2,0)\). One of the deformation coordinate is the separation distance \(R = z_1 - z_2\) In addition we can define the charge and mass asymmetries of the final products:

\[
\eta_A = \frac{A_d - A_e}{A_d + A_e}, \quad \eta_z = \frac{Z_d - Z_e}{Z_d + Z_e}
\]

(1)

Here e and d reffer to emitter (lighter) and daugther (heavier) fragments. The nuclear surface is described by the following equation:

\[
\rho(z) = \begin{cases}
\rho_1(z) = \sqrt{b_1^2 - \chi_1 z^2}, & -a_1 \leq z \leq z_{c1} \\
\rho_2(z) = \sqrt{b_2^2 - \chi_2(R - z)^2}, & z_{c1} \leq z \leq z_{c2} \\
\rho_3(z) = \rho_3 - \sqrt{R^2 - (z - z_3)^2}, & z_{c2} \leq z \leq R + a_2
\end{cases}
\]

(2)

where the origin is placed in the center of heavy fragment \(O_1\). So, the free parameters to describe the shape for the fission process are \(b_2\) (small semiaxes of the light fragment), the two ratio of ellipsoids semiaxes \(\chi_1 = b_1/a_1\), \(\chi_2 = b_2/a_2\) and \(R\).

2.2. THE MACROSCOPIC ENERGY

The core of this method is the calculation of two major parts of the total deformation energy: the macroscopic energy, obtained within the assumption of the charged liquid drop object subject to the fissionlike geometric evolution, and the microscopic part, due to the influence of the changes in the total single particle level schemes in their path from one single potential towards the two splitted potential wells.

The macroscopic energy is defined as [3]:

\[
E_{macro} = (E_s - E_s^0) + (E_c - E_c^0) = E_s^0[B_s - 1 + 2X(B_c - 1)]
\]

(3)
where \( E_s \) is the nuclear surface energy and \( E_C \) is the Coulomb part. One has to mention that compared to the complete known Weizsaecker formula, the other terms are missing since the nuclear and electrostatic terms are the only ones which are influenced by the deformation of the nucleus. In order to work with the deformation part of the energies, the two terms are scaled to the spherical shape values: 

\[
E_s^0 = a_s(1 - \kappa I^2)A^{2/3}
\]

for the surface term, and 

\[
E_c^0 = a_cZ^2A^{-1/3}
\]

for the Coulomb part. The relative energies \( B_s = E_s/E_s^0 \) and \( B_c = E_c/E_c^0 \) are functions only of the geometry of the nuclear shapes. The electrostatic energy of a charge distribution, where \( \rho_e \) is the charge density in nuclear volume \( V_n \), is:

\[
E_c = \frac{1}{8\pi} \int_{V_n} E^2(r)d^3r = \frac{1}{2} \int_{V_n} \rho_e(r)V(r)d^3r
\]

\( V(r) \) is a solution of the Poisson differential equation:

\[
\nabla^2 V = -4\pi\rho_e(r)
\]

The binary type formula for the Coulomb part reads:

\[
E_c = \frac{1}{2} \int_{V_n} \int \frac{\rho_e(r)\rho_e(r_1)d^3r^3r_1}{|r-r_1|}
\]

A folded Yukawa-plus-exponential potential is used instead of surface energy because these deficiencies: The leptodermous expansion validated just if the dimensions of the drop are large in compared to the surface thickness (condition doesn’t satisfy the strongly neck-in configurations). Also the attraction between separated nuclei at a small distance within the range of nuclear forces was absent, and the the surface diffusivity was neglected. Due to these reasons the exponential terms takes into account the finite range of the nuclear force through the “a” parameter (\( a = 0.68 \text{fm} \)). Finally we get for the Yukawa-plus-exponential energy:

\[
E_Y = -\frac{a_2}{8\pi^2r_0^2a^4} \int_{V_n} \int \frac{(r_{12}/a - 2)}{|r_1 - r_2|} \frac{\exp(-r_{12}/a)}{u} d^3r_1 d^3r_2
\]

The summation of Yukawa and Coulomb energies results in the macroscopic energy. The first and the third terms are the self-energies of each fragments and the middle one is the interaction energy between the two fragments. The relative
$Y + EM$ energies are expressed by triple integrals:

$$B_{Y1} = b_Y \int_{x_c}^{x_e} dx \int_{-1}^{1} dw F_1 F_2 Q_Y;$$

(10)

$$B_{Y2} = b_Y \int_{x_c}^{x_e} dx \int_{-1}^{1} dw F_1 F_2 Q_Y$$

$$B_{Y12} = b_Y \int_{x_c}^{x_e} dx \int_{-1}^{1} dw F_1 F_2 Q_Y$$

(11)

$$B_{c1} = b_c \int_{-1}^{x_c} dx \int_{x_c}^{x_e} dx' F(x,x');$$

(12)

$$B_{c2} = b_c \int_{x_c}^{1} dx \int_{x_c}^{1} dx' F(x,x')$$

(13)

where F (x,x) is shape dependent. The results of the macroscopic energy calculation are shown in Figs. 1 and 2 for $^{235}$U and $^{244}$Pu respectively for fission channels around magic numbers $Z = 50$ and $Z = 82$ families. The goal was to browse the Sn and Pb valleys as possible emitted fragments.

2.3. DEFORMED TWO-CENTER SHELL MODEL

The two center shell model is a very specialized microscopic model designed to describe the transition from one (parent nucleus) to two independent level schemes (daughter and emitted fragment). It was first developed by the Frankfurt school [4, 5], mainly for spherical shapes. The newest version, applicable for deformed nuclei and including the neck parameter in the proper way, has been published in [6]. It is the model that is employed in this work, being able to give solutions for extreme mass asymmetries. Total Hamiltonian is:

$$H_{DTCSM} = -\frac{\hbar^2}{2m_0} \nabla^2 + V_{DTCSM}(\rho,z) + V_{\Omega s} + V_{\Omega p}^2$$

(14)

with the two partially overlapped Nilsson potentialis:

$$V_{DTCSM}(\rho,z) = \begin{cases} V_1(\rho,z) = \frac{1}{2} m_0 \omega_1^2 \rho^2 + \frac{1}{2} m_0 \omega_2(z + z_1)^2 , & z \leq 0 \\ V_2(\rho,z) = \frac{1}{2} m_0 \omega_2 \rho^2 + \frac{1}{2} m_0 \omega_2^2 (z - z_2)^2 , & z \geq 0 \end{cases}$$

(15)

In order to separate the Hamiltonian, one considers an intermediary potential $V^d(\rho,z)$ where: $\omega_{\rho 1} = \omega_{\rho 2} = \omega_1$, and the Hamiltonian can be diagonalized for:

$$V^d(\rho,z) = \begin{cases} V_1^d(\rho,z) = \frac{1}{2} m_0 \omega_1^2 \rho^2 + \frac{1}{2} m_0 \omega_2 (z + z_1)^2 , & z \leq 0 \\ V_2^d(\rho,z) = \frac{1}{2} m_0 \omega_1^2 \rho^2 + \frac{1}{2} m_0 \omega_2 (z - z_2)^2 , & z \geq 0 \end{cases}$$

(16)
The general expression of the matrix elements of the Hamiltonian is:

\[
<i | H_{DTCSM} | j> = E^{\text{osc}}_{\text{osc}} + <i | \Delta V_1 | j> + <i | \Delta V_2 | j> + <i | \Delta V_{\Omega_1} | j> + <i | \Delta V_{\Omega_2} | j>
\]  
(17)

The second and the third terms in the matrix elements represent the difference operator between the real DTCSM potential and the diagonalized potential. The final result for the oscillator energy of the system is taken as:

\[
E_{DTCSM} = \hbar \omega_1 (2\eta_0 + | m | + 1) + \hbar \omega_{z+1} (\eta_z + 0.5)
\]
(18)

where \( \eta_z \) is no more an integer during the partially overlapped stage of the nuclei. To this energy one adds the spin-orbit and the \( l^2 \) energies, obtained from the total diagonalization of the respective potentials. The diagonalization of the intermediary...
potential results in the basis in cylindrical coordinates. The binary character of fission is given by the formula of the $Z_{\nu}$-function:

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} \exp(im\phi),$$  \hspace{1cm} (19)

$$R_{n_{\nu}}|m| = \left( \frac{2\Gamma(n_{\rho}+1)\alpha_1^2}{\Gamma(n_{\rho}+|m|+1)} \right)^{\frac{1}{2}} \exp\left(-\frac{\alpha_1^2\rho^2}{2}\right)(\alpha_1^2\rho^2)^{|m|}L_{n_{\rho}}|m|(\alpha_1^2\rho^2)^{|m|},$$  \hspace{1cm} (20)

$$Z_{\nu}(z) = \begin{cases} C_{\nu 1} \exp\left[-\frac{\alpha_1^2(z+z_1)^2}{2}\right]H_{\nu 1}[-\alpha_1(z + z_1)], & z \leq 0 \\ C_{\nu 2} \exp\left[-\frac{\alpha_1^2(z-z_2)^2}{2}\right]H_{\nu 2}[\alpha_2(z - z_2)], & z \geq 0 \end{cases}$$  \hspace{1cm} (21)

As the deformation goes from the parent nucleus to the two intersected fragments the $z$-quantum number is no more an integer.
The spin-orbit and $l^2$-operators are expressed in the creation and anihilation part functions:

\[ l_s \to \Omega s = \frac{1}{2}(\Omega^+ s^- + \Omega^- s^+) + \Omega_z s_z, \]  

\[ l^2 \to \Omega^2 = \frac{1}{2}(\Omega^+ \Omega^- + \Omega^- \Omega^+) + \Omega_z^2 \]  

The binary character of the process is included in the frequency and center position dependence of these operators:

\[ \Omega^+(\nu_1) = -e^{i\nu}[m_0\omega^2 \rho \frac{\partial}{\partial z} - m_0\omega^2 (z + z_1) \frac{\partial}{\partial \rho} - \frac{i}{\rho} m_0\omega^2 (z + z_1) \frac{\partial}{\partial \varphi}], \]  

\[ \Omega^-(\nu_1) = e^{-i\nu}[m_0\omega^2 \rho \frac{\partial}{\partial z} - m_0\omega^2 (z + z_1) \frac{\partial}{\partial \rho} + \frac{i}{\rho} m_0\omega^2 (z + z_1) \frac{\partial}{\partial \varphi}], \]  

\[ \Omega_z(\nu_1) = -i m_0\omega^2 \rho \frac{\partial}{\partial \varphi} \]  

The shape dependence relation reads:

\[ m_0\omega^2_n = \left(\frac{a_i}{b_i}\right)^2 m_0\omega^2_n, \quad m_0\omega^2_z = \left(\frac{b_i}{a_i}\right)^2 m_0\omega^2_0. \]  

As a result of diagonalization of DTCSM potential the level schemes are obtained for every distances between centers. In the figs. 3 and 4 the single-particle energies are calculated for neutron and proton separately.

3. SHELL CORRECTION (STRUTINSKY METHOD)

The shell correction is obtained by Strutinsky method [7] as the difference between the sum of the levels and the smoothed part of the microscopic energies. It was used in different publications related to the fission process [8–10]

\[ \delta u(n, \varepsilon) = \sum_{i=1}^{n} 2\varepsilon_i(\varepsilon) - \tilde{u}(n, \varepsilon) \]  

where the smooth part $\tilde{u}$ is obtained by a level smearing procedure leading to:

\[ \tilde{u} = \frac{\tilde{U}}{\hbar \omega^2_0} = 2 \int_{-\infty}^{\lambda} \tilde{g}(\varepsilon)e^{i\varepsilon} \]  

where $\tilde{g}$ is the smoothed level density. This shell correction was calculated for neutron and proton separately and after that the total shell correction is obtained by their summation.

\[ \delta E = \delta u_n + \delta u_p \]
Fig. 3 – The two level schemes for fission. These calculations were done for neutron and proton in the $^{236}\text{U}$ fission channels.

The final deformation energy will be the sum of the liquid drop (macroscopic) and shell correction (microscopic) energies:

$$E_{def} = E_{LDM} + \delta E.$$  \hspace{1cm} (31)

The variation of the shell corrections with the splitting deformation during the fission process is presented in figures 5 and 6.

3.1. PENETRABILITIES

The penetrabilities are calculated using the usual WKB approximation:

$$P = \exp(-K_{ov})$$  \hspace{1cm} (32)
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The overlaping action integral $K_{ov}$ is obtained with the total deformation energy along the whole range of the distance between centers:

$$K_{ov} = \frac{2}{\hbar} \int_{R_i}^{R_t} \sqrt{2B(R)E_{def}(R)} dR$$

(33)

where $E_{def}(R)$ is the total deformation energy, and $B(R)$ is the contracted scalar tensor of inertia. We used the Werner-Wheeler procedure to obtain the mass parameters.

4. RESULTS

The results are summarized in tables 1 and 2 for different fission channels for $^{236}$U and $^{244}$Pu respectively.
Fig. 5 – The shell correction as a function of the distance between centers up to the touching point. The calculation was done for neutron and proton separately in different fission channels around magic numbers 50 and 82 for $^{236}\text{U}$.

The most favourable fission channels corresponding to the highest penetrability value have been selected. The upper part of the figure 5 presents the neutron (δ$E_{\text{neutron}}$), proton (δ$E_{\text{proton}}$) and their sum δ$E$ for three fission channels belonging to the quasisymmetric valley of Sn emission: $Z=50-2$, 50, 50+2. One can observe the deep negative value of the proton shell correction energy especially for Sn, due to the closeness of the magic proton shell. Its influence is still strong for Te (50-2). The lower part of the figure displays the same parent U and the asymmetric fission channels. One can observe the strong influence of the Pb nucleus, Z=82 proton shell.
Fig. 6 – Same as Fig. 5 for the $^{244}$Pu fission channels.

Table 1

The quasi-symmetric and asymmetric fission channels around magic numbers 50 and 82 for $^{235}$U.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$E_b$(MeV)</th>
<th>$\ln(p)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{208}$Pb + $^{25}$Ne</td>
<td>20.674</td>
<td>-6.5614</td>
</tr>
<tr>
<td>$^{208}$Hg + $^{28}$Mg</td>
<td>18.532</td>
<td>-6.6541</td>
</tr>
<tr>
<td>$^{208}$Pt + $^{28}$Si</td>
<td>16.989</td>
<td>-4.0434</td>
</tr>
<tr>
<td>$^{120}$Te + $^{116}$Zr</td>
<td>7.455</td>
<td>-2.7376</td>
</tr>
<tr>
<td>$^{120}$Sn + $^{116}$Mo</td>
<td>12.163</td>
<td>-4.9012</td>
</tr>
<tr>
<td>$^{120}$Cd + $^{116}$Ru</td>
<td>15.090</td>
<td>-4.8982</td>
</tr>
</tbody>
</table>
Fig. 7 – Fission barriers for favourable quasisymmetric (upper plot) and asymmetric channels for the fission of $^{236}\text{U}$.

### Table 2

<table>
<thead>
<tr>
<th>Reaction</th>
<th>$E_b$(MeV)</th>
<th>$\ln(p)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{208}\text{Po} + ^{36}\text{Ne}$</td>
<td>8.824</td>
<td>−1.8691</td>
</tr>
<tr>
<td>$^{209}\text{Pb} + ^{36}\text{Mg}$</td>
<td>13.887</td>
<td>−5.9497</td>
</tr>
<tr>
<td>$^{208}\text{Hg} + ^{36}\text{Si}$</td>
<td>26.123</td>
<td>−8.5016</td>
</tr>
<tr>
<td>$^{124}\text{Te} + ^{120}\text{Mo}$</td>
<td>7.401</td>
<td>−2.7550</td>
</tr>
<tr>
<td>$^{124}\text{Sn} + ^{120}\text{Ru}$</td>
<td>9.963</td>
<td>−4.6463</td>
</tr>
<tr>
<td>$^{124}\text{Cd} + ^{120}\text{Pd}$</td>
<td>12.941</td>
<td>−5.3310</td>
</tr>
</tbody>
</table>

as negative proton shell corrections.

The same study has been made for Pu fission channels, in figure 6. Again the negative energy value of the proton shell $Z=50$ is visible in the upper part of the figure. Also this influence is still strong for its neighbours, the emission of Te and Cd. For the asymmetric channels, again the Pb valley impose its influence both for
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Fig. 8 – Same as Fig. 7 for the $^{244}$Pu fission channels.

The proton $Z=82$ and neutron $N=126$ close shells, with deep negative values of the shell corrections.

The corresponding fission barriers are displayed in figures 7 for the main fission channels of $^{238}$U around two proton magic numbers of the emitted fragment: $Z=50$ (the Sn valley) and $Z=82$ (the Pb valley). The typical two-hump barrier can be observed for quasisymmetric channels. Also the exit from the barrier is obtained beyond the touching point. Much higher barriers are obtained for the asymmetric fission channels, despite the strong influence of the Pb magicity. The values are around 20 MeV, whereas for the symmetric case they are around 15 MeV.

The corresponding penetrability values are written down in Table 1 for U and Table 2 for Pu. It is obvious that symmetric channels are favoured, with 1 to 3 order of magnitude higher values of penetrability. The most probable fission channel from $^{238}$U seems to be the emission of $^{120}$Te.

The results of the same study made for $^{244}$Pu is presented in figure 8. The lowest barrier can be observed for the emission of $^{124}$Te in the quasisymmetric val-
ley and the emission of $^{35}$Ne in the asymmetric part. The most improbable fission channel seems to be the cluster emission of $^{36}$Si.

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