

Effect of Inertia Parameters on Static Fission Path

R. A. M. S. NAZARETH

Instituto de Física, Universidade Federal do Rio de Janeiro

and

T. KODAMA

Centro Brasileiro de Pesquisas Físicas

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Properties of static (minimum potential) fission path in the formalism of Hofmann are investigated. It is pointed out that the inertial parameters greatly affect the fission path and hence the penetrability. The difficulty of determining fission path is discussed.

São investigadas as propriedades da trajetória estática (potencial mínimo) de fissão. É assinalado que os parâmetros de inércia afetam fortemente a trajetória de fissão e conseqüentemente a penetrabilidade. É discutida a dificuldade em determinar a trajetória de fissão.

The most traditional and conventional way of calculating the spontaneous fission probability is to apply the WKB approximation along a suitable fission path when the potential surface is given as a function of collective parameters (one dimensional calculation). However it has been emphasized that the degrees of freedom which are perpendicular to fission path are important even in the adiabatic fission process as well, as in the case of heavy ion reactions. In order to take these effects into account, several attempts have been made to calculate the barrier penetrability in more than one dimension¹⁻⁴. Hofmann suggested to

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apply the formalism of scattering theory to treat the transitions of states which belong to degrees of freedom perpendicular to the fission path.

Let us write the collective Hamiltonian as

$$H = -\frac{\hbar^2}{2} \frac{1}{\sqrt{M}} \frac{\partial}{\partial q^i} M^{ij} \sqrt{M} \frac{\partial}{\partial q^j} + V(q^1, q^2) \quad (1)$$

where q^1, q^2 are collective coordinates, M^{ij} the contravariant components of the inertia tensor (M_{ij}), M the determinant of M_{ij} , and V the potential.

The essential point of Hofmann's theory is to introduce a new set of coordinates

$$\begin{aligned} x &= x(q^1, q^2) \\ y &= y(q^1, q^2) \end{aligned} \quad (2)$$

which diagonalizes the inertia tensor, and then expand the potential around $y = 0$.

In the case of static fission ($(\partial V / \partial y)|_{y=0} = 0$ for all x), the new coordinates should satisfy the following two conditions

$$M^{1,1} \frac{\partial x}{\partial q^1} \frac{\partial y}{\partial q^1} + M^{1,2} \left(\frac{\partial x}{\partial q^1} \frac{\partial y}{\partial q^2} + \frac{\partial x}{\partial q^2} \frac{\partial y}{\partial q^1} \right) + M^{2,2} \frac{\partial x}{\partial q^2} \frac{\partial y}{\partial q^2} = 0$$

(diagonalization)

(3)

and

$$\left. \left(\frac{\partial V}{\partial q^1} \frac{\partial q^1}{\partial y} \right)_x + \left(\frac{\partial V}{\partial q^2} \frac{\partial q^2}{\partial y} \right)_x \right|_{y=0} = 0$$

(minimum potential)

(4)

Now let us choose

$$y = q^2 - f(q^1) \quad (5)$$

which defines the static fission path $q^2 = f(q^1)$. ^{**}

Substituting the relations

$$\left\{ \begin{array}{l} \left(\frac{\partial q^1}{\partial y}\right)_x = - \left(\frac{\partial x}{\partial q^2}\right) q^1 / \frac{\partial(x,y)}{\partial(q^1,q^2)} , \\ \left(\frac{\partial q^2}{\partial y}\right)_x = + \left(\frac{\partial x}{\partial q^1}\right) / \frac{\partial(x,y)}{\partial(q^1,q^2)} , \\ \left(\frac{\partial y}{\partial q^2}\right) = 1 , \end{array} \right. \quad (6)$$

and

$$\frac{\partial y}{\partial q^1} = - \frac{df}{dq^1}$$

into Eqs. (3) and (4) we get

$$\frac{df}{dq^1} = \frac{M^{22} \frac{\partial V}{\partial q^2} + M^{12} \frac{\partial V}{\partial q^1}}{M^{11} \frac{\partial V}{\partial q^1} + M^{12} \frac{\partial V}{\partial q^2}} \quad (7)$$

Equation (7) is the differential equation which determines the static fission path.

In fact, for the case $M^{11} = M^{22}$ and $M^{12} = 0$, Eq.(7) reduces to

$$\frac{df}{dq^1} = \left(\frac{\partial V}{\partial q^2}\right) / \left(\frac{\partial V}{\partial q^1}\right)$$

whose direction coincides with $\text{grad } V$.

** We may choose ymore generally as $y = g(q^2 - f(q^1))$ where $g(s)$ is an arbitrary function which satisfies $g(0) = 0$. Even in this case the result (Eq.(7)) is invariant.

Equation (7) manifests clearly the effect of inertia tensor on the static fission path. It is interesting to note that the equation does not have any degree of freedom for choosing the initial conditions. In other words, the initial condition is uniquely determined by the physical requirement that the minimum potential trajectory should pass on the saddle point, since otherwise the trajectory does not go over the barrier from one side to the other.

At the saddle point ($\partial V/\partial q^1 = \partial V/\partial q^2 = 0$), the potential has the form

$$V(q^1, q^2) \approx V_0 + a(q^1 - q_0^1)^2 + 2b(q^1 - q_0^1)(q^2 - q_0^2) + c(q^2 - q_0^2)^2 \quad (8)$$

where q_0^1 and q_0^2 are coordinate values of the saddle point, and a, b, c constants. (It is always possible to express the potential in the form of Eq. (8) for arbitrary q^1 and q^2 if we let a, b and c be functions of q^1 and q^2).

Introducing the new variables

$$\begin{aligned} \xi_1 &= q^1 - q_0^1 \\ \xi_2 &= q^2 - q_0^2 \end{aligned}$$

we have

$$\frac{df}{d\xi_1} = \frac{M^{22}(b\xi_1 + c\xi_2) + M^{02}(a\xi_1 + b\xi_2)}{M^{00}(a\xi_1 + b\xi_2) + M^{02}(b\xi_1 + c\xi_2)} \quad (9)$$

In the limit of $\xi_1 \rightarrow 0$, we should have $d\xi_2/d\xi_1 \rightarrow \xi_2/\xi_1$ so that we get

$$a = \frac{M^{22}(b + c\alpha) + M^{02}(a + b\alpha)}{M^{00}(a + b\alpha) + M^{02}(b + c\alpha)} \quad (10)$$

where $\alpha = \left. \left(\frac{d\xi_2}{d\xi_1} \right) \right|_{\xi_1=0}$.

Solving Eq.(10) with respect to a , we get

$$\alpha_{\pm} = \frac{(G - J) \pm \sqrt{(G - J)^2 + 4KH}}{2K} \quad (11)$$

where

$$H = M^{22}b + M^{02}a$$

$$G = M^{22}c + M^{02}b$$

$$J = M^{00}a + M^{02}b$$

$$K = M^{00}b + M^{02}c$$

Again in the case of isotropic inertia tensor ($M^{11} = M^{22}$, $M^{12} = M^{21} = 0$), the direction of the derivatives coincides with the principal axis of the potential surface, where the positive sign corresponds to the path which climbs up the potential surface and the negative sign goes down along the potential valley. Of course the latter trajectory is of our interest which connects the saddle point and the minimum of the potential.

Around the minimum, the potential can be expanded again in the following form:

$$V \approx \alpha(q^1 - q_m^1)^2 + 2\beta(q^1 - q_m^1)(q^2 - q_m^2) + \gamma(q^2 - q_m^2)^2 \quad (12)$$

where q_m^1 and q_m^2 are coordinates of the minimum. The form of the trajectory drastically changes around the minimum depending on the relative magnitudes of the coefficients α , β and γ . If the minimum is isotropic ($\beta = 0$, $\alpha = \gamma$) and the inertia tensor is not diagonal, then the trajectory forms a spiral which falls into the minimum turning it around. Such an example is shown in Fig. 1, whose static potential path is very unrealistic.

If the minimum is not isotropic, there exist again only two possible directions of the trajectory into the minimum, i.e. the two principal axis of the potential surface. However there are infinitely degenerated trajectories to these two directions at the minimum so that it is not adequate to solve Eq. (9) starting from the minimum.

In Fig. 2 we showed another example of the trajectory for the liquid drop potential of ^{240}Pu given by Brack *et al.*⁵. It is found that

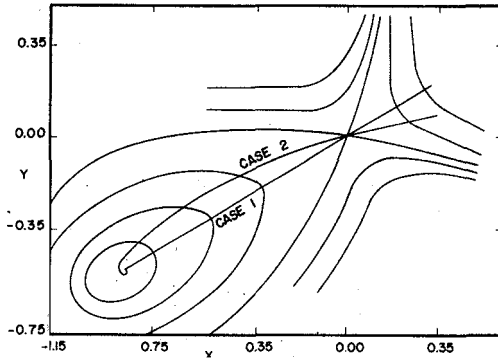


Fig.1 - Example of the static fission path for the potential $V = \frac{3}{2} (\frac{\sqrt{3}}{2}x - \frac{1}{2}y)^2 - (\frac{1}{2}x + \frac{\sqrt{3}}{2}y)^2 (\frac{1}{2}x + \frac{\sqrt{3}}{2}y - \frac{3}{2})$. The minimum of this potential is located at $x_m = -\frac{\sqrt{3}}{2}$, $y_m = -\frac{1}{2}$. The two trajectories correspond to the following inertia parameters: case 1: $M^{11} = M^{22} = 1$, $M^{12} = M^{21} = 0$, case 2: $M^{11} = M^{22} = 1$, $M^{12} = M^{21} = 0.75$.

the differential equation is not always stable for the numerical procedure near the saddle point.

Hofmann showed that the degree of freedom perpendicular to the fission path decreases the penetrability compared to the one-dimensional calculation due to the transitions among the states which belong to this degree of freedom. In addition to this, the static fission path defined by Eqs. (3) and (4) is in general much longer than the usual minimum potential path so that this also decreases the penetrability.

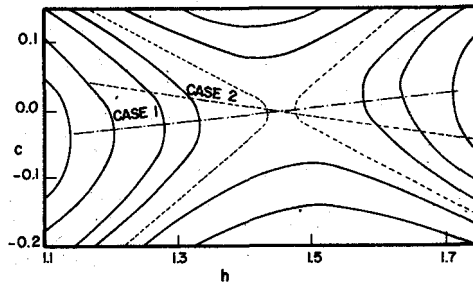


Fig.2 - Static fission path for ^{240}Pu . The potential surface is taken from Brack et al.⁵, simulated by the form,

$$V = A(c, h) (h - h_0)^2 + 2B(c, h) (h - h_0) (c - c_0) + C(c, h) (c - c_0)^2,$$

where A, B, and C are quadratic functions of c and h. The inertia parameters for trajectories case 1 and case 2 are equal to that of Fig.1.

It should be noted that, depending on the inertial parameter, the static fission path in this formalism is not adequate as seen in Fig. 1. Hofmann formulated his theory for the case that the fission path does not coincide with the minimum of the potential. However, in such a case, there should be a constant outflow of the flux from the path due to the transitions, so that the concept of the fission path becomes somewhat ambiguous.

Thus it is quite difficult to decide the fission path when the inertia coupling is very strong, although in this case we expect a considerable decrease of penetrability compared to the one dimensional calculation.

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