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Generalization of Kramers's formula: Fission over a multidimensional potential barrier

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We generalize Kramers's rate expression for diffusion over a potential barrier to the case of a diffusion problem for n degrees of freedom. These can be thought of as the shape degrees of freedom of a fissioning nucleus. We present our formula for the fission width and discuss its dependence on the parameters—the mass tensor, the friction tensor, and the shape of the potential landscape.

[NUCLEAR REACTIONS, FISSION Diffusion, transition state method.]

Kramers[1] modeled the induced nuclear fission process as a one-dimensional diffusion process over the fission barrier. He solved the Fokker-Planck equation for one degree of freedom in the quasistationary approximation. For the fission width Γ_f, he obtained the formula

$$\Gamma_f=\frac{\hbar}{2\pi}\exp\left(-\frac{V_B}{T}\right)\left(\frac{W}{|V|}\right)^{1/2}\lambda \ . \tag{1}$$

Equation (1) is obtained by calculating the quasistationary probability current over the saddle point. In Eq. (1), V_B is the height of the fission barrier, T is the nuclear temperature (in units of energy), and $W>0$ and $V<0$ are the frequencies of the parabolic potentials osculating the fission potential around the ground state and at the top of the barrier, respectively. The constant λ is the positive root of the quadratic equation

$$M\lambda^2+\beta\lambda+V=0 \tag{2}$$

where M is the mass associated with the fission variable and $\beta>0$ the friction constant [in units (mass) (time)$^{-1}$]. The value of λ decreases monotonically with increasing β and has the range

$$0\leqslant\lambda\leqslant(|V|/M)^{1/2} \text{ for } \infty>\beta\geqslant 0 \ . \tag{3}$$

The result (1) is valid for all but very small values of β, where Γ_F should depend linearly on β. Equations (1)–(3) are interpreted as follows. The fission rate is mainly determined by the exponential which reflects the Boltzmann factor, and thus the diffusive character of the process. The factor $(W/|V|)^{1/2}\lambda$ can also be written in the form $(W/|M|)^{1/2}\alpha$ where $\alpha^2+(\beta/M|V|)\alpha=1$ with $\alpha=1$ for $\beta=0$. The factor $(W/M)^{1/2}$ is the frequency in the first well, or the frequency of attempts to cross the barrier. For $\beta\neq 0$, the factor $\alpha<1$, and this frequency is reduced because of friction. The friction is expressed in terms of the dimensionless quantity $\beta/M|V|$.

Kramers's result can be generalized to a diffusion problem in n dimensions. This is desirable as several degrees of freedom are necessary to describe the shape deformations occurring during the fission process.[2] We accordingly model induced nuclear fission in terms of a Fokker-Planck equation for n degrees of freedom. This equation contains[3] the real, symmetric, and positive definite mass tensor M, the real, symmetric, and positive friction tensor β, and the potential energy $\mathscr{V}$, a function of the n position variables. Solving this equation in the quasistationary approximation, we find for the fission width the expression

$$\Gamma_f=\frac{\hbar}{2\pi}\exp\left(-\frac{V_B}{T}\right)\left(\frac{\det W}{|\det V|}\right)^{1/2}\Lambda \ . \tag{4}$$

Here, the real, symmetric, and positive definite n by n matrix W_{ij} $(i,j=1,\ldots,n)$ defines the quadratic form which osculates the fission potential $\mathscr{V}$ at the ground-state deformation of the fissioning nucleus, a local minimum of the potential landscape. The real, symmetric n by n matrix V_{ij} affords the same approximation at the saddle point. The existence of a saddle is ascertained by the fact that V has $(n-1)$ positive and one negative eigenvalues. The symbols V_B and T have the same meaning as in Eq. (1), and Λ is the only positive root of the equation

$$\det(M\Lambda^2+\beta\Lambda+V)=0 \ . \tag{5}$$

The value of Λ decreases monotonically with increasing strength β_0 of the friction tensor, and Λ has the range

$$0\leqslant\Lambda\leqslant|\phi_1|^{1/2} \ . \tag{6}$$

Here, ϕ_1 is the only negative eigenvalue of the n by n matrix $(M^{-1/2}VM^{-1/2})$. The validity of Eqs. (4) to (6) is again restricted to a domain excluding very small values of β.

Because of possible applications in several areas of statistical mechanics, the proof of Eqs. (4) to (6) will be published elsewhere.[3] In this Rapid Communication, we discuss in which way the fission width for an n-dimensional fission problem differs from Kramers's original expression (1).

The presentation just given emphasizes the very close formal analogy between the one-dimensional and the n-dimensional cases. The determining factor for both is the exponential, which is identical in both cases. Modifications of the value of Γ_f arise, however, because the last two factors on the right-hand side (rhs) of Eqs. (1) and (4) are different. We now discuss these factors.

Denoting the n eigenvalues of W_{ij} by $W_i>0$, $i=1,\ldots,n$, those of V_{ij} by V_i, $i=1,\ldots,n$ with $V_1<0$, $V_l>0$ for $l\geqslant 2$, we write the ratio of determinants as

$$\left(\frac{\det W}{|\det V|}\right)^{1/2}=\left(\frac{W_1}{|V_1|}\right)^{1/2}\prod_{i=2}^{n}\left(\frac{W_i}{V_i}\right)^{1/2} \ . \tag{7}$$

To facilitate the comparison between Eqs. (1) and (4) we assume that the major axes have been chosen in such a way that $W = W_1$ and $V = V_1$. The difference between the one-dimensional and the n-dimensional cases is then given by the product of all the $(W_i/V_i)^{1/2}$ for $i \geq 2$. This has a simple geometrical interpretation: If the n-dimensional fission valley gets wider (narrower) as one approaches the saddle point, the fission width in n dimensions is bigger (smaller) than in one dimension. This is intuitively expected. Note that actually one only compares the width of the valley at the ground state with the width of the valley at the saddle point, and that values at intermediate points are of no importance. Note also that it does not matter whether the major axes of W_{ij} are tilted as compared with those of V_{ij}, and whether the fission valley winds its way up to the scission point or runs in a straight line. These statements are, of course, expected for a diffusion process.

The value of Λ is determined exclusively by the characteristics of the problem near the saddle point, as is shown by the defining Eq. (5). We study the parameter dependence of Λ by restricting ourselves to the case of two dimensions, $n=2$. Introducing the matrices $\gamma = M^{-1/2}\beta M^{-1/2}$ and $\phi = M^{-1/2}VM^{-1/2}$, which are both real and symmetric (γ is also positive definite while ϕ has[3] one negative eigenvalue $\phi_1 < 0$ and one positive eigenvalue $\phi_2 > 0$), we write Eq. (5) in the form

$$\det(\Lambda^2 + \gamma\Lambda + \phi) = 0 \ . \tag{8}$$

Without loss of generality we can assume γ to be diagonal. Our problem contains the five parameters $\gamma_1 > 0$, $\gamma_2 > 0$ (the eigenvalues of γ), $\phi_1 < 0$, $\phi_2 > 0$ (the eigenvalues of ϕ), and the angle θ of the real orthogonal 2 by 2 matrix which diagonalizes ϕ. We define $\bar{\Lambda} = \Lambda/|\phi_1|^{1/2}$ and are then left with four parameters. These are conveniently chosen as the dimensionless quantities

$$\begin{aligned} &\eta = \gamma_1/|\phi_1|^{1/2} \geq 0, \quad R_\gamma = \gamma_2/\gamma_1 \geq 0 \ , \\ &R_\phi = \phi_2/|\phi_1| \geq 0, \quad \xi = \cos^2\theta + R_\gamma \sin^2\theta \ . \end{aligned} \tag{9}$$

[Equation (8) can be seen to depend on θ only via the function $\sin^2\theta$. Therefore we consider only the interval $0 \leq \theta \leq \pi/2$. In this interval, the correspondence between ξ and θ is one to one.]

These parameters can be interpreted as follows. The quantity ϕ_1 is the curvature of V at the fission saddle in the direction of steepest descent, modified by the geometry imposed by M. The angle θ is the angle of rotation that takes the major axes of the friction tensor into those of the potential at the saddle, again in the "deformed" geometry implied by the mass tensor M. The parameters R_γ, R_ϕ, and η defined in Eqs. (9) have an obvious interpretation, while ξ measures the strength of friction (in units of γ_1) in the direction of steepest descent.

We note that η also determines, in the case of $n=1$, the parameter dependence of

$$\bar{\lambda} = \lambda/|\phi_1|^{1/2} = (\lambda/V_1|^{1/2})M^{1/2} \ .$$

Indeed, we have

$$\bar{\lambda} = [1 + (\eta/2)^2]^{1/2} - \eta/2 \ . \tag{10}$$

In contradistinction, the other three parameters R_γ, R_ϕ, and ξ are typical for $n=2$ and do not occur for $n=1$. The parameter ξ equals unity unless $R_\gamma \neq 1$. This makes sense since, for $R_\gamma = 1$, the matrix γ is a multiple of the unit matrix, and γ and ϕ can then be diagonalized simultaneously. Denoting the left-hand side (lhs) of the eigenvalue equation (8) by $D(\Lambda)$, we use[3] that $dD/d\Lambda > 0$ for $\Lambda > 0$. Moreover, the eigenvalue equation (8) can for $n=2$ be written as

$$(\bar{\Lambda}^2 + \eta\bar{\Lambda} + \bar{\phi}_{11})(\bar{\Lambda}^2 + \eta R_\gamma \bar{\Lambda} + \bar{\phi}_{22}) = \bar{\phi}_{12}^2 \ , \tag{11}$$

where $\bar{\phi}_{ik} = \phi_{ik}/|\phi_1|$. For $\phi_{12} \neq 0$, the two factors on the lhs of Eq. (11) have the same sign. This sign is positive. Indeed, for $R_\gamma = 1$, we have $\bar{\Lambda} = \bar{\lambda}$, and the positivity follows from Eq. (10) and direct calculation. For $R_\gamma \neq 1$ the claim follows from the continuity of $\Lambda(R_\gamma)$ in R_γ and the fact that the rhs of Eq. (11) is positive and independent of R_γ. Using these inequalities and the eigenvalue equation (8), it is straightforward to show that

$$\frac{\partial\bar{\Lambda}}{\partial R_\gamma} < 0; \quad \frac{\partial\bar{\Lambda}}{\partial R_\phi} < 0; \quad \frac{\partial\bar{\Lambda}}{\partial \xi} < 0 \ . \tag{12}$$

The derivatives are taken by keeping the other parameters (9) fixed. The second of these inequalities shows that making the fission valley steeper (or the mass tensor smaller) in a direction different from the direction of steepest descent reduces $\bar{\Lambda}$ and thus Λ. To discuss the first inequality, we consider a change of R_γ in (9) by keeping γ_1 fixed and increasing γ_2. To keep ξ fixed, we decrease (or increase) at the same time the angle θ depending on whether $R_\gamma > 1$ ($R_\gamma < 1$). (Unfortunately, this interdependence of the variables required to keep γ_1 and ξ fixed complicates the discussion.) Under this transformation, $\bar{\Lambda}$ (and thus Λ) is reduced. This is intuitively reasonable: The increase of R_γ (γ_1 fixed) implies an increase of γ_2 and, hence, an overall increase of friction which reduces Λ. The fact that θ is changed simultaneously does not affect the conclusion. The third inequality is similarly discussed: For $R_\gamma > 1$, i.e., $\gamma_1 > \gamma_2$, the maximum of γ is attained for $\theta = \pi/2$, i.e., when the 1-axis of ϕ and the 2-axis of γ are made to coincide. for $R_\gamma < 1$, i.e., $\gamma_2 < \gamma_1$, we have analogously $\theta = 0$. In both cases, the fission width is minimized by maximizing the friction along the direction of steepest descent.

To discuss, finally, the dependence of $\bar{\Lambda}$ on η, we recall that $\bar{\lambda}$ also depends on η, and that we are primarily interested in changes caused by the multidimensionality of the problem. We therefore consider the quantity $\bar{\Lambda}/\bar{\lambda} = \Lambda/\lambda$ and find after some algebra

$$\frac{\partial}{\partial\eta}\left(\frac{\bar{\Lambda}}{\bar{\lambda}}\right) \begin{cases} > 0 & \text{if } 1 > R_\gamma \ , \\ = 0 & \text{if } 1 = R_\gamma \ , \\ < 0 & \text{if } 1 < R_\gamma \ . \end{cases} \tag{13}$$

Since $\bar{\Lambda} = \bar{\lambda}$ for $R_\gamma = 1$, this implies $\bar{\Lambda} < \bar{\lambda}$ ($> \bar{\lambda}$) for $R_\gamma > 1$ (< 1), respectively. These results again are intuitively obvious: An increase of friction implies a decrease of Λ.

Figure 1 shows the parameter dependence of Λ/λ calculated for various values of the parameters. We see that Λ/λ can differ from unity by a factor of 2 or so in either direction.

In conclusion, we have presented a modified version of Kramers's formula which includes the effects of several collective degrees of freedom on the fission width. We have shown that such effects may substantially modify the fission width, although the original formula of Kramers gives a

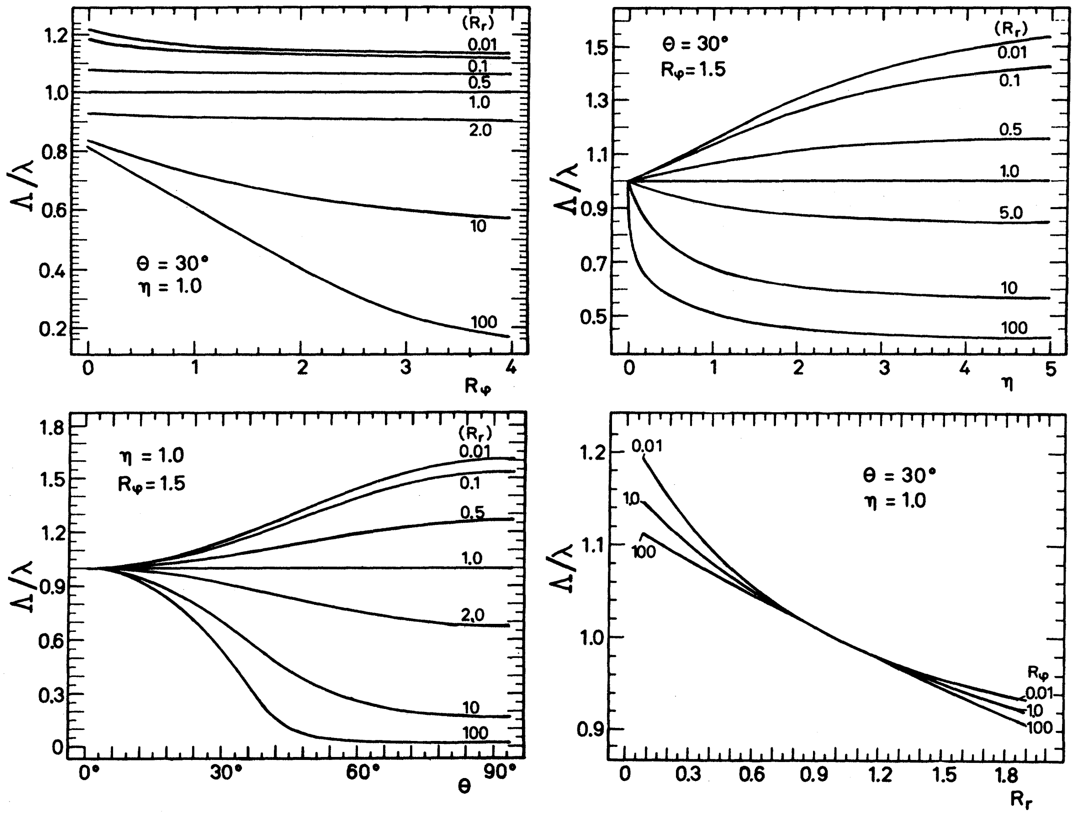

FIG. 1. The ratio Λ/λ for $n=2$ plotted vs each of the four parameters η, R_γ, R_ϕ, and θ, for various values of the remaining parameters as indicated.

correct order-of-magnitude estimate. The modifications are intuitively understandable in terms of the shape of the fission valley, the two eigenvalues of the friction tensor, and the skewness of the direction of the fission current as compared with the direction of steepest descent over the saddle.

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