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Fission Probability Calculation by Solving Fokker-Plank Equation with Variation Method

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A variation method is developed to solve the Fokker-Planck (F-P) equation. One-dimensional fission probability is calculated and compared with other methods. The relation of the F-P equation and the Smoluchowski equation is discussed in light of this method, which paves the way to derive the multi-dimensional Smoluchowski equation with varying mass and viscosity and to solve more complicated equations.

Key words: variation method, Fokker-Plank equation, probability of fission.

1. INTRODUCTION

The study of fission with Browning motion model can be reduced to solving the Fokker-Plank (F-P) equation. Many works have been done [1-4] in this direction. For the difficulties of solving the F-P equation, most of the published works are limited to the one-dimensional case and variations of the inertia and dissipation with nuclear deformation are neglected. In a former work [5], we have treated the two-dimensional fission problem by direct solving the Langevin equation with Monte Carlo method and calculated the variation of inertia and dissipation with deformation. Such an approach relies crucially on the dynamical behavior of the nuclear system. It is both difficult and unreliable, since the dynamical behaviors of the fissioning system are not clearly understood. For large dissipations, velocity distributions of the system can be considered as nearly Maxwellian distribution

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and the F-P equation can be reduced to the Smoluchowski (Smo.) equation. Some of the fission studies are performed by solving the Smo. equation [6-8]. The derivation of the Smo. equation from the F-P equation is usually done for the one-dimensional case with constant inertia and dissipation. How to obtain the Smo. equation in the general multidimensional case with variable inertia and dissipation tensors? Which terms are neglected in the Smo. equation in comparison with the F-P equation? These problems await future study. In this work, a variational method is developed to solve the one dimensional F-P equation, and fission probabilities are calculated using the same model potential as in [1] and [4]. The results are in general agreement with the numerical solution in [1] and the Monte Carlo method in [4]. The relation between the F-P equation and the Smo. equation is also studied. Solving the multidimensional F-P equation with variable inertia and dissipation tensors and deriving the Smo. equation in the general case are in progress with the same variational procedure.

2. THEORETICAL FORMULATION

The F-P equation is a non self-adjoint linear differential equation. Ordinary variational method cannot be applied. Extended variational method has been discussed in general principles [11]. In the following, we give a brief description of the application of variation principle to the F-P equation.

For the sake of simplicity, the one-dimensional F-P equation is considered,

$$\frac{1}{\tau_0}\frac{\partial W}{\partial t} = -v\frac{\partial W}{\partial x} + \frac{\partial U}{\partial x}\frac{\partial W}{\partial v} + \beta\left[\frac{\partial}{\partial v}(Wv) + \frac{\partial^2 W}{\partial v^2}\right], \tag{1}$$

where kT is the unit of potential U, kT/m is the unit of velocity v, m denotes inertia parameter, time unit $t_0 = 10^{-21}$ s, and length unit $l = 1.16 \times 10^{-13}$ cm. Then the parameters τ_0 and β in Eq. (1) are given by

$$\tau_0 = \frac{t_0}{l}\sqrt{\frac{kT}{m}}, \quad \beta = \frac{l\alpha}{m}\sqrt{\frac{m}{kT}}, \tag{2}$$

where α is the coefficient of viscosity. Let

$$W = Ae^{-\tau_0\omega t}F, \tag{3}$$

then Eq. (1) can be reduced to the form of eigenequation,

$$\hat{L}F = \omega F, \tag{4}$$

$$\hat{L} = v\frac{\partial}{\partial x} - \frac{\partial U}{\partial x}\frac{\partial}{\partial v} - \beta\left[1 + v\frac{\partial}{\partial v} + \frac{\partial^2}{\partial v^2}\right]. \tag{5}$$

Assuming $U \to \infty$ as $x \to \pm\infty$ and F is quadratically integrable in the whole x, v region, we can define $\hat{L}^+$ as the adjoint operator of $\hat{L}$ by the following relation

$$\int \psi_1 \hat{L}\psi_2 d\tau = \int \psi_2 \hat{L}^+ \psi_1 d\tau, \tag{6}$$

where ψ_1 and ψ_2 are any two quadratically integrable functions and $d\tau = dvdx$. Take the functional $I(F,G)$ as

$$I(F,G) = \int \Phi G \hat{L} F \mathrm{d}\tau, \tag{7}$$

where Φ is an arbitrary function. To find the extreme value of I by variation under the condition

$$\int \Phi F G \mathrm{d}\tau = 1. \tag{8}$$

We shall introduce ω as the Langrangian multiplier and write I as

$$I(F,G) = \int \Phi G \hat{L} F \mathrm{d}\tau - \omega \int \Phi F G \mathrm{d}\tau. \tag{9}$$

By variation with respect to G, we obtain

$$\frac{\delta I}{\delta G} = \Phi \hat{L} F - \omega \Phi F = 0 \quad \hat{L} F = \omega F, \tag{10}$$

in agreement with Eq. (4). Using formula (6), (9) can be changed to

$$I(F,G) = \int F \hat{L}^{+} \Phi G \mathrm{d}\tau - \omega \int \Phi F G \mathrm{d}\tau.$$

By variation with respect of F, we obtain

$$\frac{\delta I}{\delta F} = \hat{L}^{+} \Phi G - \omega \Phi G = 0 \quad \hat{L}^{+} \Phi G = \omega \Phi G. \tag{11}$$

Using the definition (6) of the adjoint operator, after suitable partial integration, we obtain from Eq. (5) the adjoint operator of $\hat{L}$

$$\hat{L}^{+} = -v \frac{\partial}{\partial x} + \frac{\partial U}{\partial x} \frac{\partial}{\partial v} + \beta \left(v \frac{\partial}{\partial v} - \frac{\partial^2}{\partial v^2} \right). \tag{12}$$

Taking

$$\Phi = \mathrm{e}^{U(x)} \mathrm{e}^{v^2/2}, \tag{13}$$

we obtain

$$\hat{L}^{+} \Phi G = \Phi \left[-v \frac{\partial}{\partial x} + \frac{\partial U}{\partial x} \frac{\partial}{\partial v} - \beta \left(1 + v \frac{\partial}{\partial v} + \frac{\partial^2}{\partial v^2} \right) \right] G$$

$$\equiv \Phi \hat{L}' G.$$

Formula (11) now becomes:

$$\hat{L}' G = \omega G. \tag{14}$$

Comparing $\hat{L}'$ and $\hat{L}$, we find $\hat{L}'(-v,x) = \hat{L}(v,x)$, and formula (14) becomes

$$\hat{L}(v,x)G(-v,x) = \omega G(-v,x). \tag{15}$$

Comparing with Eq. (10), we get

$$G(-v,x) = F(v,x). \tag{16}$$

Let ω_1, ω_2, $\cdots$ be a series of eigenvalues of Eq. (4), then from Eqs. (10) and (11), we have

$$\hat{L}F_i = \omega_i F_i, \quad \hat{L}^+ \Phi G_j = \omega_j \Phi G_j,$$

hence

$$\int \Phi G_j \hat{L} F_i \mathrm{d}\tau = \omega_i \int \Phi G_j F_i \mathrm{d}\tau,$$

$$\int F_i \hat{L} \Phi G_j \mathrm{d}\tau = \omega_j \int F_i \Phi G_j \mathrm{d}\tau.$$

From the relation of adjoint operators (6), the left side of the above equations are equal, hence $(\omega_i - \omega_j) \oint \phi F_i G_i = 0$ when $i \neq j$. Combining with the normalization condition (8), we have the orthogonality and normalization condition

$$(\omega_i - \omega_j) \int \Phi F_i G_j = 0$$

$$\iint \Phi(x,v) F_i(x,v) G_j(x,v) \mathrm{d}x\mathrm{d}v = \delta_{ij}, \tag{17}$$

which must be satisfied by the eigenfunctions.

Corresponding to the eigenvalue $\omega_0 = 0$, the eigenfunction F_0 must be the equilibrium solution of the F-P equation. It is easy to see from the eigenequation that

$$F_0(x,v) = B\mathrm{e}^{-U(x)}\mathrm{e}^{-v^2/2}, \tag{18}$$

where B is a constant. The general solution W can be written as

$$W(x,v,t) = A_0 F_0(x,v) + \sum_{j=1} A_j \mathrm{e}^{-\tau_0 \omega_j t} F_j(x,v), \tag{19}$$

where constant A_0 and A_1 can be determined by the conditions imposed on W at $t \to \infty$ and $t \to 0$. For $t \to \infty$, one obtains from the normalization condition,

$$A_0 = \frac{1}{\iint_{-\infty}^{\infty} F_0(x,v)\mathrm{d}x\mathrm{d}v}. \tag{20}$$

For the initial condition, let us assume that at $t = 0$, the system stays at the deformation $x = 0$ with a Maxwellian distribution for velocities, then from Eq. (19), we obtain

$$A_0F_0(x,v) + \sum_{j=1} A_jF_j(v,x) = \frac{1}{\sqrt{2\pi}} e^{-v^2/2}\delta(x). \tag{21}$$

Here, we have chosen the initial valley of potential to be at $x = 0$ and $U(0) = 0$, hence

$$\Phi(x = 0, v) = e^{v^2/2}. \tag{22}$$

Multiplying $\Phi F_j(x, -v)$ to both side of Eq. (21) and integrating over $d\tau$, we get

$$A_j = \frac{1}{\sqrt{2\pi}} \int F_j(x = 0, -v)dv, \tag{23}$$

Fixing A_0 and A_j, we obtain the solution of the F-P equation

$$W = \frac{e^{-U}e^{-v^2/2}}{\iint_{-\infty}^{\infty} e^{-U}e^{-v^2/2}dxdv} + \sum_{j=1} A_j e^{-\omega_j t}F_j. \tag{24}$$

To calculate the eigenvalue ω_j and the corresponding eigenfunctions, we shall first expand $F(x,v)$ as a function of v in terms of weighted Hermit polynomials $H_{e,n}(v)$:

$$F(x, v) = \sum_{m=0} e^{-U/2}e^{-v^2/2}(2\pi)^{-\frac{1}{4}} \frac{1}{\sqrt{m!}} H_{e,m}(v)\phi_m(x). \tag{25}$$

We substitute Eq. (25) into Eq. (9) and perform the integration over v with the help of relations between Hermite polynomials, then the functional can be expressed in terms of $\phi_n(x)$

$$I = \sum_{n=0} (-1)^n \int \phi_n(x)[2\sqrt{n+1}J_-\phi_{n+1}(x) + (\beta_n - \omega)\phi_n(x)]dx, \tag{26}$$

where

$$J_- = \frac{d}{dx} - \frac{1}{2}\frac{dU}{dx}, \quad J_+ = \frac{d}{dx} + \frac{1}{2}\frac{dU}{dx}. \tag{27}$$

From

$$\frac{\delta I}{\delta \phi_0} = 0$$

one get

$$J_-\phi_1 - \omega\phi_0 = 0, \tag{28}$$

and from

$$\frac{\delta I}{\delta \phi_1} = 0$$

one obtains

$$J_+\phi_0 + \sqrt{2}J_-\phi_2 + (\beta - \omega)\phi_1 = 0. \tag{29}$$

Neglecting ϕ_2 and eliminating ϕ_1 from Eq. (28) and Eq. (29), one obtains

$$J_-J_+\phi_0 + (\beta - \omega)\omega\phi_0 = 0, \tag{30}$$

where $J_-J_- = \dfrac{d^2}{dx^2} + \left[\dfrac{1}{2}\dfrac{d^2U}{dx^2} - \dfrac{1}{4}\left(\dfrac{dU}{dx}\right)^2\right]$. If ω in the factor $(\beta - \omega)$ of the above formula is neglected, Eq. (30) reduced to the one dimensional Smo. equation. From Eq. (2) one knows that β is proportional to the viscosity coefficient α and ω is the eigenvalue of Eq. (4). From Eq. (18), it is clear that for not very small t values, contributions of the larger ω_j to W are negligible. Hence for sufficiently large viscosity, it is reasonable to neglect ω in the factor $\beta - \omega$. This derivation shows that we can obtain the Smo. equation from the F-P equation by expanding $F(x,v)$ in Hermit polynomials, keeping only $n = 0$ and 1 terms and neglecting ω compared with β. The multi-dimension Smo. equation with variable inertial and dissipation tensors can be derived in a similar manner.

To solve the F-P equation. $\phi_n(x)$ in Eq. (26) can be expanded also in terms of Hermit polynomials,

$$\phi_n(x) = \sum_{s=0} \alpha_{ns}\phi_s(x), \tag{31a}$$

$$\phi_s(x) = \sqrt{\frac{1}{\sqrt{\pi}\,2^s s!}}\, H_s(x)e^{-x^2/2}. \tag{31b}$$

Thus, after performing the integration in Eq. (26) with respect to x, we can express I in a quadratic form of the expansion coefficients α_{ns}. Taking $n = 0, 1, \cdots (r-1)$, and $s = 0, 1, \cdots (q-1)$, we obtain r×q linear equations from $\partial I/\partial\alpha_{ns}$. The solution of these equations yields both the eigenvalues ω_j and the corresponding eigenfuctions F_j. An approximate solution of the F-P equation is thus obtained.

3. RESULTS OF CALCULATION

Since the object of this work is to study the method of solving the F-P equation for fission problems, we shall use the simple potential energy form as given in [1] and [4].

$$U = G[x^4 + a_1x^3 + a_2x^2 + a_3x + a_4] + H, \tag{32}$$

with constants $G = 0.0089366$, $H = 3.816$, $a_1 = 28.328$, $a_2 = 121.587$, $a_3 = 0.3729$, $a_4 = -427.05$. The initial valley lies at $x = 0$ with $U = 0$, the barrier peak $U = 3.816$ lies at $x = x_c = 3.41$ and a very deep valley $U = -193.92$ lies at $x = 17.84$, with kT being the unit of U. Fission takes place whenever the model particle crosses over the barrier. Let $J(t)$ be the probability for the particle to remain inside the barrier at time t, then

$$J(t) = \int_{-\infty}^{x_c} dx \int_{-\infty}^{\infty} dv W(x,v,t), \tag{33}$$

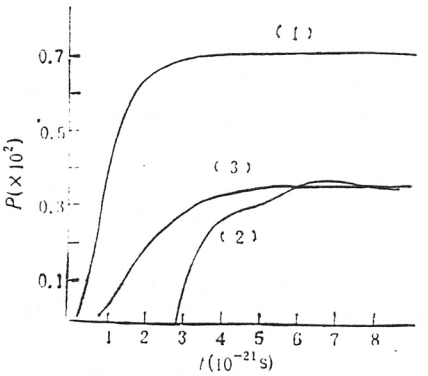

Fig. 1
Change of fission probability with time t (unit 10^{-21} s).

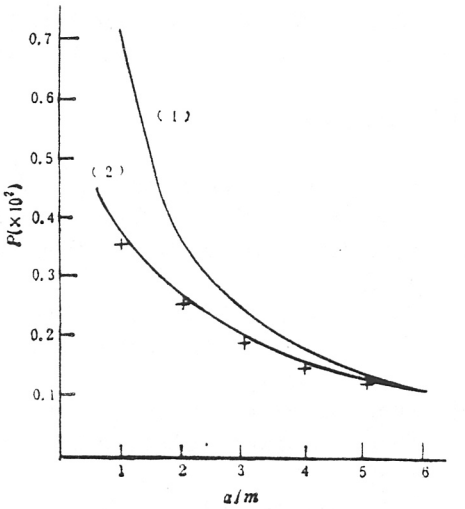

Fig. 2
Change of stationary fission probability P with the viscosity coefficient α.

and the fission probability P is given by

$$P = -\frac{1}{J}\frac{dJ}{dt}. \tag{34}$$

We take the mass number $A = 248$ and $\alpha/m = 1, 2, \cdots, 6$ etc., where m denotes the mass of the fissioning nucleus. It is found that 7 to 9 terms are sufficient for velocity expansion and 25 terms are enough for each $\phi_1(x)$. The calculated results are show in Figs. 1 and 2. In Fig. 1, the fission probability is exhibited as a function of t for $\alpha/m = 1$. In this figure, curve 1 is the solution of the Smo. equation, curve 2 is the solution of the F-P equation. It is shown that the difference between the two solutions is rather large. For large matrices (e.g., dimensions 225×225), many of the eigenvalues are complex, which leads to oscillating fission probabilities for small t. In curve 2, the oscillating part is simply omitted. The resulting curve approaches to the numerical solution of [1]. We have also taken average value for the oscillating part, and curve 3 is obtained in this way. Results obtained with Monte Carlo method in [4], coincide essentially with curve 3. In Fig. 2, the stationary values of fission probabilities are plotted against α/m. Curve 1 is the value obtained from the Smo. equation and curve 2 is obtained from the F-P equation. The values obtained from the Smo. equation approach those of the F-P equation only for $\alpha/m \geq 6$. In the figure, points marked with "+" are corresponding to values obtained from Kramers' formula

$$P' = \frac{\omega_A}{4\pi\omega_c\tau}\left[\sqrt{1 + 4\tau^2\omega_c^2} - 1\right]e^{-H_0/kT}. \tag{35}$$

where ω_A and ω_c are oscillating frequencies at the equilibrium point and at the saddle point (inverse frequency). This indicates that for stationary fission probabilities, Kramers' formula is a simple and rather accurate formula.

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