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Study of the Multidimensional Kramers Equation

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The position of saddle point and potential energy surface near the saddle point are studied for a given fissioning system. Multidimensional inertia and viscosity tensors are calculated with both irrotational flow and Werner-Wheeler approximation, and the fission rate is calculated with multidimensional Kramers formula. It is found that the fission rate increases reasonably with the number of dimensions considered and changes only slightly with the assumptions used in kinetic energy calculations. The results of calculations indicate that a suitable three-dimensional calculation will be sufficient to yield accurate fission rates.

Key words: multidimensional potential energy surface, inertia and viscosity, Kramers formula, fission rate.

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1. INTRODUCTION

The Kramers formula has special significance in fission studies. Its result can either be used as a reference in the stationary state for other approaches [1,2], or as stationary initial conditions for the calculations of fission mass distributions and other fission properties [3,4]. In those studies, one-dimensional results were usually adopted. This is obviously insufficient. In 1980, we derived a general multidimensional Kramers formula [5], and Zhuo Yizhong *et al.* obtained the two-dimensional formula [6]. In 1984, Weidenmuller and coworkers presented a more elegant multidimensional Kramers formula [7]. Since then, the multidimensional formula has been applied to the calculation of

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the fission rate, but whether the fission probability is increased or decreased when the number of dimensions is increased has not been solved [8-11]. In some publications the effect of quantum corrections on fission rates were studied, and it was found that the effect is not serious at the reasonable higher excitation energies [12,13], where the Kramers formula is applicable. The purpose of this work is to compare the fission rates calculated with the different numbers of dimensions and to determine the reasonable number of dimensions necessary for the accurate calculation of fission rates. In this paper, the potential energy surface of the nucleus ^{213}At is calculated with two kinds of deformation parametrizations in one, two, three and four dimensions. The inertia tensors are calculated by using both Werner-Wheeler method and irrotational fluid model [14]. The viscosity tensor is evaluated in terms of the one-body dissipation mechanism [15]. It is found that the fission barrier decreases with the increasing number of dimensions. When the number of dimensions increases. The elongation of the nucleus at the saddle point increases slightly and the fission rates increase reasonably with two sets of deformation parameters and two methods the resultant inertia tensors are quite different, but the resultant fission rates only differ slightly. It seems that the adoption of deformation parameters (c,h,α) yield a reasonable fission rate with less effort.

2. FORMULA AND RESULTS

2.1. Fission Rate Formula

Weidenmuller's multidimensional fission rate formula can be written as

$$R = (H/2\pi)\{(\det\overline{W})/|\det\varphi|\}^{1/2}\exp(-U/kT), \tag{1}$$

where R is the fission rate and $\bar{W}$ is the reduced potential energy tensor, namely,

$$\det\overline{W} = (\det W)/(\det M_0). \tag{2}$$

Let $x_1, x_2, \ldots, x_n$ stand for a set of deformation parameters. In the vicinity of the spherical shape, the potential energy surface V and the kinetic energy E_k can be written in the following forms:

$$V = (1/2)\Sigma W_{ij}x_i x_j, \tag{3}$$

$$E_k = (1/2)\Sigma M_{0ij}\dot{x}_i\dot{x}_j. \tag{4}$$

Note the M_0 is the inertia tensor of the spherical nucleus. In [7], it was incorrectly pointed as the saddle-point inertia tensor. By using Eq. (2), Eq. (1) completely agrees with the rate formula given in [5]. In [8] one has realized the mistake in [7]. In Eq. (1), U is the barrier height at the saddle point and T is nuclear temperature. In the calculation kT is taken to be 1 MeV and

$$\det(\varphi) = \det(V)/\det(M), \tag{5}$$

where M is the inertia tensor at the saddle point. In the vicinity of the saddle point, the potential and kinetic energies are given by:

$$V = U + (1/2)\Sigma V_{ij}x_i x_j, \tag{6}$$

and

$$E_k = (1/2)\Sigma M_{ij}\dot{x}_i\dot{x}_j. \tag{7}$$

where $x_1, x_2, \ldots, x_n$ are measured from the saddle point. H is the only positive solution of the equation

$$\det\begin{pmatrix}\gamma + HI & -I \\ \varphi & HI\end{pmatrix} = 0, \tag{8}$$

where I is the unit tensor, Z denotes the viscosity tensor at the saddle point and γ and ϕ are given by

$$\gamma = (M^{1/2})Z(M^{1/2}). \tag{9}$$

2.2. Calculation of Potential Energy

Potential energy is calculated with the finite range liquid drop model[16]. Using the (c,h,α) parametrization, the equation of the nuclear surface is given by

$$\rho^2 = (c^2 - z^2)(A + Bz^2/c^2 + \alpha z/c + Dz^4/c^4), \tag{10}$$

where one more parameter D is introduced to enlarge the deformation degrees of freedom. To keep the volume unchanged during the deformation, A and B in Eq. (10) is connected with the deformation parameters by

$$A = 1/c^3 - 0.4h - 0.1(c-1) - 6D/70, B = 2h + 0.5(c-1). \tag{11}$$

The position of the saddle point on the potential energy surface and the barrier height U are given in Table 1. It is noted from this table that the introduction of the parameter D considerably affects the position of the saddle point and the barrier height.

Four-dimensional potential energy tensor V and W defined by Eqs. (6) and (2) are:

$$V = \begin{array}{c} \begin{array}{cccc} c & h & \alpha & D \end{array} \\ \begin{pmatrix} -97.70 & -73.55 & 0.00 & -23.61 \\ -73.55 & 178.29 & 0.00 & 28.57 \\ 0.00 & 0.00 & 487.37 & 0.00 \\ -23.60 & 28.57 & 0.00 & 14.95 \end{pmatrix} \end{array}, W = \begin{array}{c} \begin{array}{cccc} c & h & \alpha & D \end{array} \\ \begin{pmatrix} 137.51 & 36.58 & 0.00 & 11.10 \\ 36.58 & 35.26 & 0.00 & 7.39 \\ 0.00 & 0.00 & 15.45 & 0.00 \\ 11.10 & 7.39 & 0.00 & 2.39 \end{pmatrix} \end{array}.$$

When the equation of the nuclear surface is expressed in spherical coordinates r and Θ, the surface equation can be expanded by spherical harmonics:

$$r = \lambda R f(x), x = \cos(\theta), \tag{12}$$

and

$$f(x) = 1 + a_2P_2(x) + a_3\psi_3(x) + a_4P_4(x) + a_6P_6(x), \tag{13}$$

where a_2, a_3, a_4, a_6 are deformation parameters, $P_i(x)$ denotes the spherical harmonics, ψ_3 is given in Eq. (15) and λ is introduced to keep the volume conservation. By using the same model as before, the position of the saddle point and barrier height are given by

$$a_2 = 0.830283, \ a_3 = 0, \ a_4 = 0.262604, \ a_6 = -0.027689, \ U = 9.840840. \tag{14}$$

Comparing the barrier heights calculated from two different parametrizations, it can be seen that the results with three parameters (c,h,α) are almost equivalent to those with four parameters (a_2,a_3,a_4,a_6). It this point that parametrization (c,h,α) has more advantages than the harmonic expansion. For comparison, the potential energy tensor at the saddle point and spherical nucleus are given in the following:

$$
\begin{array}{cc}
 & \begin{array}{cccc} a_2 & a_4 & a_6 & a_3 \end{array} \\
V = & \begin{pmatrix} 31.90 & -91.00 & 27.92 & 0.00 \\ -91.00 & 116.95 & -18.33 & 0.00 \\ 27.92 & -18.33 & 172.62 & 0.00 \\ 0.00 & 0.00 & 0.00 & 21.54 \end{pmatrix},
\end{array}
$$

$$
W = \begin{pmatrix} 121.32 & -0.094 & -0.088 & 0.00 \\ -0.094 & 554.73 & -0.114 & 0.00 \\ -0.088 & -0.114 & 605.39 & 0.00 \\ 0.00 & 0.00 & 0.00 & 61.68 \end{pmatrix}.
$$

2.3. Calculations of Inertia and Viscosity Tensors

Two methods are used to calculate the inertia and viscosity tensors. With (c,h,α,D) parametrization, the Werner-Wheeler method is adopted. The inertia tensor M and viscosity tensor Z at the saddle point are given in the following:

$$
\begin{array}{cc}
 & \begin{array}{cccc} c & h & \alpha & D \end{array} \\
M = & \begin{pmatrix} 10985.9 & 11418.1 & 0.000 & 3533.4 \\ 11418.1 & 13244.9 & 0.000 & 3847.7 \\ 0.000 & 0.000 & 16595.4 & 0.000 \\ 3533.4 & 3847.7 & 0.000 & 1179.3 \end{pmatrix},
\end{array}
$$

$$
Z = \begin{pmatrix} 2735.5 & 2733.3 & 0.000 & 875.22 \\ 2733.3 & 3565.8 & 0.000 & 992.76 \\ 0.000 & 0.000 & 6192.9 & 0.000 \\ 875.22 & 992.76 & 0.000 & 314.31 \end{pmatrix}.
$$

For the spherical nucleus, the inertia tensor is

$$
M = \begin{pmatrix} 3576.4 & 787.6 & 0.000 & 260.2 \\ 787.53 & 227.3 & 0.000 & 66.64 \\ 0.000 & 0.000 & 68.50 & 0.000 \\ 260.2 & 66.64 & 0.000 & 21.39 \end{pmatrix}.
$$

It should be mentioned that the units used are MeV for energy and 10^{-22} sec for time. Similar results with three parameters (c, h, α) are not presented.

When parameters a_2, a_3, a_4, a_6 are adopted, the inertia tensors are calculated in the irrotational fluid model. In order to keep the center of mass fixed during the deformation, the function $\psi_3(x)$ is defined by

$$\psi_3(x) = x^3 - (r_1/r_2)x, \tag{15}$$

where

$$r_1 = \int f^3(x)x^4\mathrm{d}x, r_2 = \int f^3(x)x^2\mathrm{d}x, \tag{16}$$

Table 1
Relation between the saddle point and the number of dimensions.

Number of dimensions and parameters	Saddle point position	Barrier height (MeV)
1 dim., c	$c = 1.74355$	$U = 10.028$
2 dim., c, α	$c = 1.74355$, $\alpha = 0$	$U = 10.028$
2 dim., c, h	$c = 1.76401$, $h = -0.034578$	$U = 9.8822$
3 dim., c, h, α	$c = 1.76401$, $h = -0.034578$, $\alpha = 0$	$U = 9.8822$
3 dim., c, h, D	$c = 1.77416$, $h = 0.000607$, $D = -0.17277$	$U = 9.7047$
4 dim., c, h, D, α	$c = 1.77416$, $h = 0.000607$, $D = -0.17277$, $\alpha = 0$	$U = 9.7047$

Table 2
Constants H and fission rates with the different set of parameters.

Number of dimensions and parameters	H	Fission rates $R(10^{16}\mathrm{s}^{-1})$
1 dim., c	0.03008	0.450
2 dim., c, α	0.03008	1.33
2 dim., c, h	0.03164	0.941
3 dim., c, h, α	0.03164	2.58
3 dim., c, h, D	0.03260	1.313
4 dim., c, h, D, α	0.03260	3.637
3 dim., a_2, a_4, a_6	0.03125	1.503
4 dim., a_2, a_4, a_6, a_3	0.03125	2.673

In this way, the deviations of the resultant a_3-related components of the inertia tensor are considerable reduced. The results of the inertia and viscosity tensors at the saddle point are given by

$$\begin{array}{cc} & \begin{array}{cccc} a_2 & a_4 & a_6 & a_3 \end{array} \\ M = & \begin{pmatrix} 2323.4 & 1262.3 & 476.3 & 0.000 \\ 1262.3 & 1601.6 & 839.7 & 0.000 \\ 476.3 & 839.7 & 809.6 & 0.000 \\ 0.000 & 0.000 & 0.000 & 268.98 \end{pmatrix}, \end{array}$$

$$Z = \begin{pmatrix} 618.8 & 223.3 & 127.9 & 0.000 \\ 223.3 & 647.3 & 321.9 & 0.000 \\ 127.9 & 321.9 & 533.3 & 0.000 \\ 0.000 & 0.000 & 0.000 & 1061.5 \end{pmatrix}.$$

and the inertial tensor for the spherical nucleus is

$$M = \begin{pmatrix} 3196.7 & 0.000 & 0.000 & 0.000 \\ 0.000 & 888.0 & 0.000 & 0.000 \\ 0.000 & 0.000 & 409.8 & 0.000 \\ 0.000 & 0.000 & 0.000 & 234.6 \end{pmatrix}.$$

2.4. Calculation of Fission Rates

With the calculated inertia and viscosity tensors, H and fission rate can be evaluated from Eqs. (4) and (1), respectively. All calculated results in various cases are presented in Table 2.

From Table 2, we see that: (1) parametrization (c,h,α) in the cylindrical coordinate system is equivalent to parametrization (a_2,a_3,a_4,a_6) in the spherical coordinate system; (2) although the inclusion of backward and forward asymmetrical deformation parameters α and a_3 does not alter the saddle point position or the barrier height, its influence on fission rate cannot be neglected; (3) for the calculation of the inertia tensor, the Werner-Wheeler method is α good approximation for deformations up to the saddle point.

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