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On Solution of the Fokker-Planck Equation for Fissioning Hot Nuclei[1]

Rozwiązanie równania Fokkera-Plancka do rozszczepiających się gorących jąder

1. INTRODUCTION

The description of the fission process by a transport equation goes back to a fundamental paper by K. Kramers [1] and has been taken up again by several authors (see e.g. [2–4]) in recent time, especially when one discovered that the transport theory was a useful tool to describe heavy-ions reactions.

It was shown in [3] that within the linear response theory the fission dynamics is governed by a generalized Fokker-Planck equation (FPE) for the distribution function $f(q,p,t)$:

$$\frac{\partial f(q,p,t)}{\partial t} = -\frac{p}{m(q)}\frac{\partial f(q,p,t)}{\partial q} + + \frac{\partial U(q)}{\partial q}\frac{\partial f(q,p,t)}{\partial p} + + \frac{\gamma(q)}{m(q)}\frac{\partial}{\partial p}[pf(q,p,t)] + D(q)\frac{\partial^2}{\partial p^2}f(q,p,t). \quad (1)$$

Here m and γ are the inertia and friction parameters respectively. U is the deformation potential which can be identified with the free energy in an adiabatic theory.

The FPE can be solved analytically in the simplest cases only. It is the case for example when the transport coefficient is constant and the

[1] This work is supported partially by CPBP 0...9.

potential U has a parabolic form. More complicated cases have to be solved numerically. We present in the next section some most frequently used numerical method of solving FPE. We shall also try to combine the Monte-Carlo random numbers procedure with the propagator method. In the next section we present the numerical results for the probability that system does not fission.

2. METHOD OF SOLVING OF FPE

The approximate solution of the FPE with the variable transport coefficient for the fission dynamics was presented in [5]. It was assumed there that the form of the distribution function $f(q,p,t)$ can be described by its first and second moments:

$$f(q,p,t) = \frac{1}{2\pi \det S} \times$$

$$\times \exp\{\frac{-S_{pp}(q-Q)^2 - 2S_{qp}(q-Q)(p-P) - S_{qq}(p-P)^2}{\det S}\} \qquad (2)$$

where Q and P are the average coordinate and momentum respectively:

$$Q(t) = \int qf(q,p,t)dqdp \qquad (3)$$

$$P(t) = \int pf(q,p,t)dqdp \qquad (4)$$

and S is the matrix of the quadratic deviation from the average values Q and P:

$$S_{qq} = \int (q-Q)^2 f(q,p,t)dqdp \qquad (5)$$

$$S_{qp} = \int (q-Q)(p-P)f(q,p,t)dqdp \qquad (6)$$

$$S_{pp} = \int (p-P)^2 f(q,p,t)dqdp \qquad (7)$$

The expression (2) is accurate for the gaussian form of the distribution function. Inserting eq. (2) into the FPE (1) one can get the coupled set of the differential equations [6] for the first:

$$\frac{\partial Q}{\partial t} = \frac{P}{m} \qquad (8)$$

$$\frac{\partial P}{\partial t} = -\frac{\partial U}{\partial Q} - \frac{\gamma}{m} P \tag{9}$$

and the second moments:

$$\frac{\partial S_{qq}}{\partial t} = \frac{2}{m} S_{qp} \tag{10}$$

$$\frac{\partial S_{qp}}{\partial t} = \frac{1}{m} S_{pp} - \frac{\partial U^2}{\partial Q^2} S_{qq} - \frac{2\gamma}{m} S_{pp} \tag{11}$$

$$\frac{\partial S_{pp}}{\partial t} = 2D - 2\frac{\partial U^2}{\partial Q^2} S_{qp} - \frac{2\gamma}{m} S_{pp} \tag{12}$$

This method is very convenient especially for the multidimensional case. The generalization of eqs (8–12) for that case is obvious [6]. But on the other side this gaussian approximation of the distribution function cannot be applied in the case of a large potential anharmonicity and variable transport coefficients.

A better, more accurate method of solving of the FPE was proposed in [7] where the propagator method was applied. Namely it was assumed there that the density probability after a small time interval Δt is done by the folding integral from the density at the time t and the propagator function K:

$$f(q,p,t+\Delta t) = \int K(q,p,t+\Delta t; q',p',t) f(q',p',t) dq dp \tag{13}$$

The propagator K was assumed to be of the gaussian form:

$$K(q,p,t+\Delta t; q',p',t) =$$

$$\frac{1}{2\pi \det S} \exp\{-\frac{S_{pp}(q-q')^2 - 2S_{qp}(q-q')(p-p') - S_{qq}(p-p')^2}{\det S}\} \tag{14}$$

where its widths S_{qq}, S_{qp} and S_{pp} are equal to zero at the initial time t (it means that K is equal to the Dirac δ-function) and they grow with increasing time according to the same equations as those for the moments of the whole distribution, eqs (8–12).

One has to repeat the process of evaluating of the folding integral (13) n times in order to get the final distribution at the time $t_n = t_o + n\Delta t$. The propagator method is accurate when the time step Δt is small enough. The numerical effort to proceed this recursive folding is very large and the calculation can be effectively done on large computers only. The

problem becomes even more complicated when we are dealing with the multidimensional collective space. This folding procedure becomes more difficult when one assumes the Gauss form of the distribution function in the moment direction. The validity of this approximation was discussed in [8].

In the present paper we propose a simplified version of the propagator method which nevertheless leads to the exact solution of FPE. Following the idea of [9] we adopt the Monte-Carlo method of generating random points on (q,p) plane to evaluate the folding integral (13).

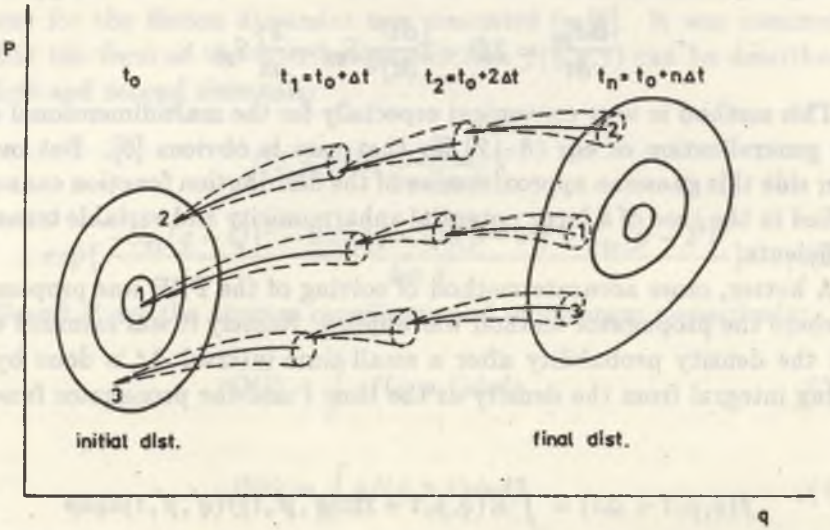

Fig. 1. The schematic illustration of the Monte-Carlo method of solving of FPE

The method of the calculation is illustrated in the graph in Fig. 1. and it is following:

1. At the initial time $t_0 = 0$ one has to generate N random points: (q_0^ν, p_0^ν), where $\nu = 1,2,\ldots N$. The distribution of these points is obtained from the initial shape of the function $f(q,p,t_0) = 0$.

2. The position (q_1^ν, p_1^ν) of each random point and its smearing width $S_{ij}^\nu(t_1)$ at the time $t_1 = t_0 + \Delta t$ is given by the solution of the coupled differential equations (8–12). The initial conditions for the widths are: $S_{qq}^\nu(t_0) = S_{qp}^\nu(t_0) = S_{pp}^\nu(t_0) = 0$

3. In the next step, at the time $t = t_1$ only one random point (q_2^ν, p_2^ν) for each trajectory ν is generated. The random number generator with the normal (gaussian) distribution described by the moments $S_{qq}^\nu(t_1), S_{qp}^\nu(t_1)$

and $S^{\nu}_{pp}(t_1)$ has to be used here. Then one repeats the procedure like in the point (2).

4. The final distribution $f(q,p,t_n)$ at the time $t_n = t_0 + n\Delta t$ is given by the end positions of the N randomly distributed points (q^{ν}_n, p^{ν}_n).

The statistical distribution will be more and more smooth with the growing number N of random points (q^{ν}, p^{ν}).

When the time interval Δt between the sequential toss is small enough one can solve the set of eqs (8–12) approximately. Namely, it is possible to assume that locally around the point q^{ν}_i the potential U is parabolic and the transport coefficients m, γ and D are constant. These approximations allow to find the analytical solutions of eqs (8–9) and eqs (10–12) which become uncoupled. The solutions of eqs (8–9) after the i-th iteration reads:

$$q^{\nu}_{i+1} = q^{\nu}_i + \left(\frac{F}{\omega^2} - \frac{A}{\alpha_1}e^{-\alpha_1\Delta t} - \frac{B}{\alpha_2}e^{-\alpha_2\Delta t}\right)/m \tag{15}$$

$$p^{\nu}_{i+1} = Ae^{-\alpha_1\Delta t} + Be^{-\alpha_2\Delta t} \tag{16}$$

where

$$F = -\frac{dU}{dq}$$

$$\omega = \sqrt{\frac{\frac{d^2U}{dq^2}}{m}}.$$

$$\alpha_1 = \frac{\gamma}{2m} + \sqrt{\left(\frac{\gamma}{2m}\right)^2 - \omega^2}$$

$$\alpha_2 = \frac{\gamma}{2m} - \sqrt{\left(\frac{\gamma}{2m}\right)^2 - \omega^2}$$

$$A = \frac{\alpha_1 p^{\nu}_i - F}{\alpha_1 - \alpha_2}$$

$$B = \frac{-\alpha_2 p^{\nu}_i + F}{\alpha_1 - \alpha_2}$$

The coupled system of eqs (10–12) for the second moments has now the following solution:

$$S_{qq}^{\nu} = \frac{D}{m^2}\{\frac{1}{\alpha_1\alpha_2(\alpha_1+\alpha_2)} - \frac{1}{(\alpha_1-\alpha_2)^2}[\frac{1}{\alpha_1}e^{-2\alpha_1\Delta t} + \frac{1}{\alpha_2}e^{-2\alpha_2\Delta t} - \frac{4}{\alpha_1+\alpha_2}e^{-(\alpha_1+\alpha_2)\Delta t}]\} \tag{17}$$

$$S_{qp}^{\nu} = \frac{D}{m(\alpha_1-\alpha_2)}[e^{-2\alpha_1\Delta t} + e^{-2\alpha_2\Delta t} - 2e^{-(\alpha_1+\alpha_2)\Delta t}] \tag{18}$$

$$S_{pp}^{\nu} = D\{\frac{1}{\alpha_1+\alpha_2} - \frac{\alpha_1\alpha_2}{(\alpha_1-\alpha_2)^2}[\frac{1}{\alpha_2}e^{-2\alpha_1\Delta t} + \frac{1}{\alpha_1}e^{-2\alpha_2\Delta t} - \frac{4}{\alpha_1+\alpha_2}e^{-(\alpha_1+\alpha_2)\Delta t}]\} \tag{19}$$

For the small time interval Δt the right hand sides of equations (15–19) can be expanded in the Taylor series:

$$q_{i+1}^{\nu} = q_i^{\nu} + \frac{p_i^{\nu}}{m}\Delta t + \frac{1}{2}(\frac{F}{m} - \frac{\gamma}{m^2}p_i^{\nu})\Delta t^2 + \frac{1}{6}[\frac{p_i^{\nu}}{m}(\frac{\gamma^2}{m^2} - \omega^2) - \frac{\gamma}{m^2}F]\Delta t^3 + ... \tag{20}$$

$$p_{i+1}^{\nu} = p_i^{\nu} + (F - \frac{\gamma}{m}p_i^{\nu})\Delta t + \frac{1}{2}[p_i^{\nu}(\frac{\gamma^2}{m^2} - \omega^2) - \frac{\gamma}{m}F]\Delta t^2 - \frac{1}{6}[\frac{\gamma}{m}(\frac{\gamma^2}{m^2} - 2\omega^2)p_i^{\nu} - (\frac{\gamma^2}{m^2} - \omega^2)F]\Delta t^3 + ... \tag{21}$$

$$S_{qq}^{\nu} = \frac{2D}{m^2}(\frac{1}{3}\Delta t^3 + ...) \tag{22}$$

$$S_{qp}^{\nu} = \frac{D}{m}(\Delta t^2 - \frac{\gamma}{m}\Delta t^3 + ...) \tag{23}$$

$$S_{pp}^{\nu} = 2D[\Delta t - \frac{\gamma}{m}\Delta t^2 + (2\frac{\gamma^2}{m^2} - \omega^2)\Delta t^3 + ...] \tag{24}$$

The terms of the order higher than 3 in Δt are neglected here.

The Fokker-Planck equation solved by the Monte-Carlo method is essentially equivalent to the Langevin equation with the normally distributed random force [10], when one omits in the equations (20–24) the terms of the order higher than 1 in Δt.

3. RESULTS OF THE CALCULATIONS

The calculation was performed for the hot, fast rotating ^{187}Ir nucleus, which was experimentally investigated in [11]. We have taken the following Ansätze for the transport parameters when solving the FPE. The fission barrier of ^{187}Ir was evaluated with the temperature dependent liquid drop parameters estimated in [12] The relative distance between fission fragments was taken as the collective coordinate and the fission barrier was minimized versus the neck parameter. We have got e.g. the fission barrier of the height $U_B = 1.41$ MeV for the nucleus temperature $T = 2.5$ MeV and the angular momentum $I = 55\hbar$. The collective inertia $m(q)$ in eq. (1) was assumed to be equal to reduced mass for relative motion of fission fragments and the friction parameter γ was taken constant and it is given by the equation

$$\beta = \frac{\gamma}{m} = 1 \cdot 10^{21} \mathrm{s}^{-1}.$$

The diffusion parameter D is related to the friction function by the Einstein relation: $D = \gamma T$.

It is not easy to compare the whole distribution functions $f(q,p,t)$ obtained by different method of solving of the FPE (1). So we have chosen a global factor related to $f(q,p,t)$

$$\mathcal{F}_{sc}(t) = \int_{-\infty}^{q_{sc}} dq\, dp\, f(q,p,t), \tag{25}$$

which gives the probability that the deformation of the nucleus is smaller than that at the scission point q_{sc}. The number of nuclei which do not fission up to the given time t is proportional to $\mathcal{F}_{sc}(t)$:

$$N(t) = N_0\, \mathcal{F}_{sc}(t), \tag{26}$$

where N_0 is the initial number of nuclei at the time $t = 0$.

We have solved the FPE within the local harmonic approximation (eqs. 15–19) and using the Monte-Carlo method. The 10 000 random points were generated. The initial shape of the distribution function $f(q,p,t)$ was taken in the form of the probability distribution of the harmonic oscillator [13] which approximates the potential $U(q)$ and mass $m(q)$ around equilibrium deformation. The probability $\mathcal{F}_{sc}$ (eq. 25) that a nucleus does not fission is plotted in Fig. 2 as a function of time. The different curves in the plot correspond to various time intervals Δt_i between the sequential toss of the random points. Here, we have taken Δt_i = (0.05, 0.1, 0.2, 0.3, 0.4, 0.5,

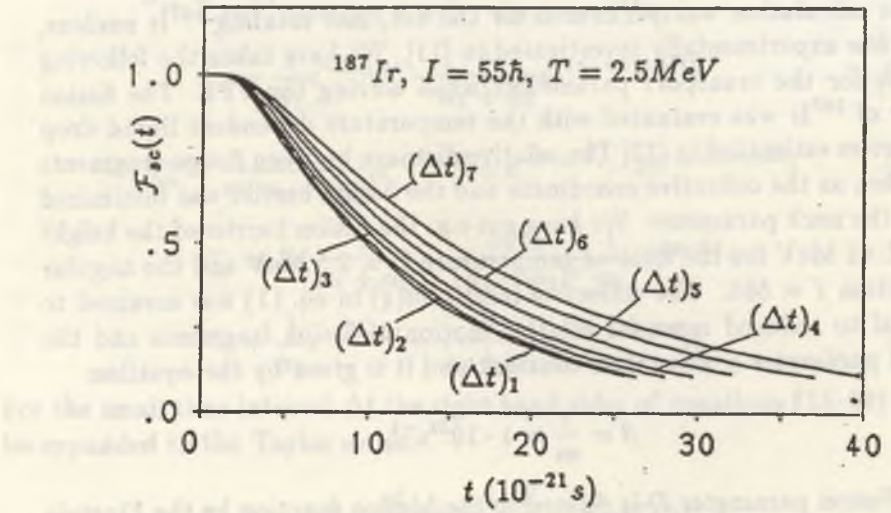

Fig. 2. The Monte-Carlo estimate of the probability $\mathcal{F}_{sc}$ (eq. 25) that a nucleus do not fission, $\Delta t_i = (0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6)10^{-21}$ s

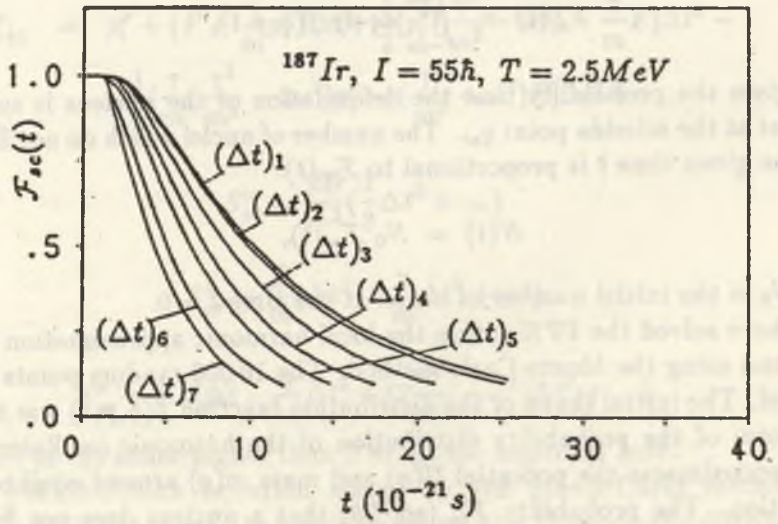

Fig. 3. The same as in Fig. 2. but for the first order in Δt expansion when solving the FPE, $\Delta t_i = (0.03, 0.05, 0.1, 0.15, 0.2, 0.3, 0.4)\cdot 10^{-21}$ s

$0.6)\cdot 10^{-21}$ s. As it is seen from the figure we have got the convergence for $\Delta t_i \leq 10^{-22}$ s.

Similar Monte-Carlo results as in Fig. 2 but for the expansion of eqs. (15–19) up to the first order terms in time are plotted in Fig. 3. Note that in this case the FPE is equivalent to the corresponding Langevin equation. We have chosen the following time intervals Δt_i = (0.03, 0.05, 0.1, 0.15, 0.2, 0.3, 0.4)$\cdot 10^{-21}$ s. The convergence was reached for $\Delta t_i \leq 0.5 \cdot 10^{-22}$ s. The results of the Monte-Carlo calculation of $\mathcal{F}_{sc}$ are compared in Fig. 4 with the exact solution (solid line) of the FPE obtained by the propagator method (eq. 13–14). The dashed line represents the results from Fig. 3 while the dotted line that from the Fig. 2. The both Monte-Carlo curves were evaluated for the time interval $\Delta T_i = 0.5 \cdot 10^{-22}$ s, while in the case of the propagator method Δt_i was four times longer.

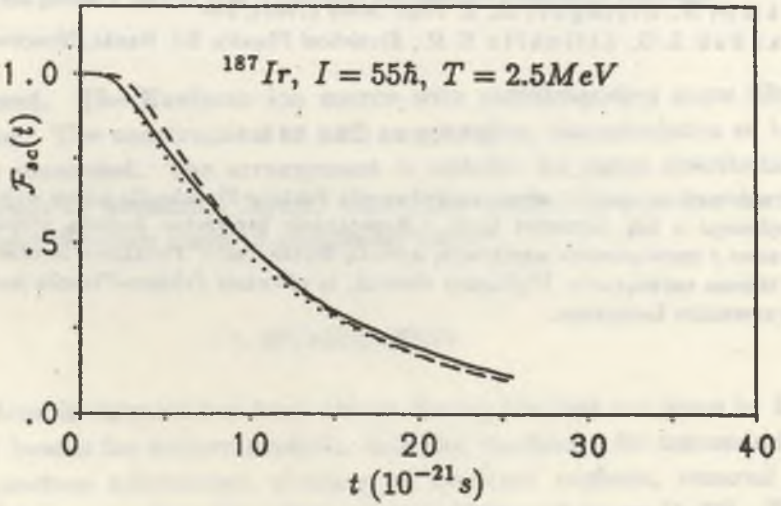

Fig. 4. The results of the Monte-Carlo calculation of $\mathcal{F}_{sc}$ compared with the exact solution (solid line) of the FPE obtained by the propagator method. The dashed line represents the results from Fig. 3 while the dotted line that from the Fig. 2

We can conclude that the the results obtained with these three methods are close to each other and that the numerical effort by the propagator method is the largest one. Additionally, we have found that this effort grows significantly with the dimension of the collective coordinates space while it is not the case for the Monte-Carlo method based on the first order expansion in Δt.

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STRESZCZENIE

Przedstawiono sposób rozwiązania równania Fokkera-Plancka dla jednej współrzędnej i sprzężonego z nią momentu pędu. Rozwiązanie otrzymane metodą propagatorów porównano z rozwiązaniem uzyskanym metodą Monte-Carlo. Pokazano, że obie metody dają zbliżone rozwiązania. Wykazano również, że równanie Fokkera-Plancka jest równoważne równaniu Langevina.