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USE OF A TRANSPORT EQUATION FOR THE DYNAMICAL BEHAVIOUR OF THE NUCLEAR FISSION

F. Scheuter and C. Grégoire
DPh-N/MF, CEN Saclay 91191 Gif-sur-Yvette, Cedex, France

Abstract

A Fokker Planck equation is used for the problem of nuclear fission. The decay rate is computed within a three dimensional calculation and the influence of coupling terms in the transport coefficient tensors is considered. Initial conditions at the saddle point for the collective degrees of freedom are dynamically obtained in the stationary situation. Finally, dynamics of fluctuations from saddle to scission is treated under the same assumptions on the propagation.

1. Introduction

Dynamical aspects of the nuclear fission could be considered in two steps, namely the path through the fission barrier and the descent from the saddle point to the scission region. On the other hand, it turns out that the coupling between the intrinsic (i.e. nucleonic) degrees of freedom and the relevant collective coordinates (i.e., in the fission problem, the elongation, the mass asymmetry and the striction) leads to a dynamical equation[1] for the density d relative to the collective space. This equation is a Fokker-Planck equation (FPE). It is a transport equation and can be applied to the two steps of the fission process. As a matter of fact, the transport equation provides some flux at the top of the fission barrier by coupling of states inside the first well. We can get a determination of the escape rate through the barrier, as far as excited nuclei are concerned. Furthermore initial conditions at the saddle point can be evaluated, starting from a statistical equilibrium in the first well. It is finally straightforward to extend the treatment from saddle to scission in order to compute macroscopic observables and the fluctuations around the mean values.

As it was already shown by F. Scheuter and H. Hofmann[2] the main difficulty for applying the FPE to the problem of the nuclear fission is due to the breakdown of the local harmonic approximation for the density d. (We will avoid here the questionable validity of the Markov approximation in the fission problem). Nevertheless use of propagators in time[2] seems to offer a way in order to solve the FPE and to treat the two steps of the nuclear fission on an equal footing. For realistic cases, conditions on the propagation make the computation tractable by introduction of propagators on gaussian bundles[3].

In this contribution, we would like to report some recent calculations obtained in a three dimensional framework. In a first part, we will give the main ideas of our dynamical calculations. In a second one, we will discuss the question of the escape rate for the multidimensional situations. In a third part, fluctuations will be considered and comparisons with some experimental results will be given.

2. Propagation on gaussian bundles

Let us write the FPE in the one-dimensional case[1], where Q is the coordinate and P the associated momentum

$$\frac{\partial d(Q,P,t)}{\partial t} = -\{d(Q,P,t), \mathcal{H}_{coll}\} + \frac{\gamma}{B}\frac{\partial}{\partial P}(P\, d(Q,P,t)) + D\frac{\partial^2}{\partial P^2} d(Q,P,t) \qquad (1)$$

$\mathcal{H}_{coll}$ is the collective hamiltonian
γ, B, D are the friction, the inertia and the diffusion coefficients and could be evaluated by li-

near response theory[1]. The resolution of this FPE proposed in ref.[2] is based on the evaluation of the propagator $K(Q,P,Q_o,P_o,t)$ defined as :

$$d(Q,P,t) = \int dQ_o\, dP_o\, K(Q,P,Q_o,P_o,t)\; d(Q_o,P_o,\, t=0) \tag{2}$$

It fulfills the relation

$$\lim_{t\to o} K(Q,P,Q_o,P_o,t) = \delta(Q-Q_o)\;\delta(P-P_o). \tag{3}$$

One can check that K satisfies the same FPE as d itself.

The initial condition (3) allows to make to local harmonic approximation for the propagator during a time interval $\Delta\tau$. According to (2), the distribution d can be reconstructed after $\Delta\tau$ and a new propagator $K^{(1)}$ can be defined as :

$$d(Q,P,\Delta\tau+t) = \int dQ_1\, dP_1\, K^{(1)}(Q,P,Q_1,P_1,\Delta\tau+t)\; d(Q_1,P_1,t). \tag{4}$$

By iteration on time, one finally gets the solution of the FPE :

$$d(Q,P,t) = \int \prod_{j=0}^{n-1} dQ_j\, dP_j\, K^{(j)}(Q_{j+1},P_{j+1},Q_j,P_j,j\Delta\tau)\; d(Q_o,P_o,t=0) \tag{5}$$

with

$$t = n\Delta\tau \text{ and } \lim_{\Delta\tau\to 0} K^{(j)}(Q_{j+1},P_{j+1},Q_j,P_j,\Delta\tau) = \delta(Q_{j+1}-Q_j)\;\delta(P_{j+1}-P_j). \tag{6}$$

Let us now add some condition on propagation[3]. As long as the potential energy and the transport coefficients are momentum independent, the collective hamiltonian can be seen as a quadratic one in momentum. Consequently, deviations from the quadratic behaviour are essentially expected in the coordinate direction. Therefore, we have assumed a gaussian momentum distribution for each given value Q_o of the coordinate. The phase space is considered as a bundle $\{Q_o, \mathcal{F}_{Q_o}\}$ where the density along each bundle is a gaussian.

This decomposition is schematically drawn in fig. 1 and can be expressed by :

$$d(Q,P,t) = \int dQ_o\, d_{red}(Q_o)\, \frac{1}{\sqrt{4\pi\omega_o}} \exp - \frac{(P-\langle P_o\rangle)^2}{4\omega_o}\, \delta(Q-Q_o) \tag{7}$$

where P_o is the local momentum for a fixed Q_o value

$$\omega_o \equiv \frac{1}{2}\int dP (P-\langle P\rangle)^2\, d(Q_o,P,t) \quad \text{the local variance}$$

$$d_{red}(Q_o) = \int dP_o\, d(Q_o,P_o,t) \quad \text{the reduced density.}$$

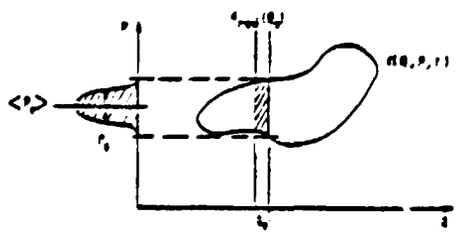

Fig. 1 : Definition of the bundled space $\{Q_o, \mathcal{F}_{Q_o}\}$. The $\mathcal{F}_{Q_o}$ is here along the momentum P and is assumed to be a gaussian.

The propagation in time is obtained in its simplified version by means of propagators on gaussian bundles $K_{bundled}$:

$$d(Q,P,t) = \int dQ_o\, K_{bundled}(Q,P,Q_o,t)\; d_{red}(Q_o) \tag{8}$$

with

$$\lim_{t\to o} K_{bundled}(Q,P,Q_o,t) = \delta(Q-Q_o)\, \frac{1}{\sqrt{4\pi\omega_o}} \exp - \frac{(P-\langle P_o\rangle)^2}{4\omega_o}. \tag{9}$$

The assumption of gaussian bundles tremendously reduces the computation of the propagation and can be extended for multidimensional purposes. As far as the fission process is concerned, the consideration of two potential regions (on one hand, the first well and the saddle point region and on the other hand, the descent from saddle to scission) permits to estimate the escape rate, the initial conditions at the saddle point and the fluctuations in the scission region.
Here, the collective coordinates[5] are the elongation c, the mass asymmetry α and a neck degree of freedom h. We assumed non diagonal inertia and friction tensors*,[5] :

$$[B] = \begin{bmatrix} B_c & B_{ch} & 0 \\ B_{hc} & B_h & 0 \\ 0 & 0 & B_\alpha \end{bmatrix} \quad \text{and} \quad [\gamma] \begin{bmatrix} \gamma_c & \gamma_{ch} & 0 \\ \gamma_{hc} & \gamma_h & 0 \\ 0 & 0 & \gamma_\alpha \end{bmatrix}$$

with

$$B_c = B_\alpha = m_o = \frac{1}{160} A^{5/3} \left[\frac{\hbar^2}{MeV}\right] , \; B_h = \frac{m_o}{1.2}$$

which are similar values as in ref.[7]
and $\gamma_c = \gamma_\alpha = f\,\gamma_o$, $\gamma_h = f\,\gamma_o/1.2$ where $\gamma_o = \frac{m_o}{\hbar}$.

The coupling terms are equal to m_o (resp. $f\,\gamma_o$) multiplied by a reduction factor.
For a given elongation value c_o, the bundle is defined like the $\{P_c,h,P_h,\alpha,P_\alpha\}$ space, where P_c (resp. P_h,P_α) is the associated momentum to c(resp. h,α).
The stationary solution of the FPE (1) provides[5] the escape rate r (or decay rate for the fissioning nucleus) according to :

$$r = \int d\Gamma_{red} ([B]^{-1} [P]\, d_{st})_{c_{saddle}} \qquad (10)$$

where $[P] = (P_c,P_h,P_\alpha)$

d_{st} the stationary solution of (1)
c_{saddle} the elongation at the saddle point
$d\Gamma_{red} = dP_c\, dh\, dP_h\, d\alpha\, dP_\alpha$.

The full distribution at the left hand side of the saddle point is assumed to be normalized to unity at each time. The half life time τ for a nucleus decaying by fission can be estimated in such a case by $\tau = 1/r$.
Since d_{st} (c_{saddle}) defines the initial conditions in the associated bundle $\mathcal{F}_{c_{saddle}}$, we are able to follow the subsequent dynamical behaviour from saddle to scission. For instance, the fluctuation $\chi^{\alpha\alpha}$ around the mean value for the mass asymmetry coordinate α gives the fluctuation for the mass ratio of the fission fragments at the scission point. Using the relationship[5] :

$$\frac{A_1}{A_2} = \frac{1 + \frac{3}{8}\alpha c^3}{1 - \frac{3}{8}\alpha c^3} \qquad (11)$$

we obtain directly :

$$\frac{\sigma_{AA}^2}{2} = \left(\frac{3}{16} A\, c^3\right)^2 \chi^{\alpha\alpha} \qquad (12)$$

if $\chi^{\alpha\alpha} = \frac{1}{\Gamma} \int d\Gamma_{red}\, (\alpha - \langle\alpha\rangle)^2 d_{red}$ at the scission point.

3. The escape rate through the fission barrier

First of all, in order to test our procedure, we studied a simple model case. We defined the po-

tential U(c,h,x) to be

$$U(c,h,x) = \begin{cases} (37.46\ (c-1)^2 + 500\ h^2 + 200\ x^2)\,[\mathrm{MeV}] & \text{for } 0 < c < 1.27 \\ (8.- 18.73\ (c-1.8)^2 + 500\ h^2 + 200\alpha^2)\,[\mathrm{MeV}] & \text{for } 1.27 < c < \infty \end{cases}$$

The coupling between c and h in the inertia and in the friction tensor is neglected in this model case ($B_{ch} = \gamma_{ch} = 0$). The nucleus under consideration is ^{205}At.

This model is for the elongation degree of freedom c essentially identical to the one dimensional model used before for the calculation of the decay rate by Kramers[3], Visscher[3] and Scheuter and Hofmann[2]. For the (h,x) degrees of freedom, we added the potentials of two harmonic oscillators with constant stiffness along c. As far as the computation of the decay rate is concerned this choice of the potential and the transport coefficients reduces the problem to the one-dimensional one studied before. The numerical results of[2,9] show that Kramers formulae[9] are virtually exact except for a very small γ-interval in the transition from the small friction (L) to the high friction regime (H). These formulae can be written in the following way :

$$r = \frac{\gamma_c}{B_c}\frac{\Omega_B}{T}\exp\left(-\frac{U_B}{T}\right) \quad \text{for} \quad \frac{\gamma_c}{B_c} \lesssim \frac{\Omega_o T}{U_B} \qquad (L)$$

$$r = \frac{\Omega_o}{2\pi\Omega_B}\left(\sqrt{\Omega_B^2 + \left(\frac{\gamma_c}{2B_c}\right)^2} - \frac{\gamma_c}{2B_c}\right)\exp\left(-\frac{U_B}{T}\right) \quad \text{for} \quad \frac{\gamma_c}{B_c} \gtrsim \frac{\Omega_o T}{U_B} \qquad (H)$$

where $\Omega_o = \left(\sqrt{\frac{\partial^2 U}{\partial c^2}/B_c}\right)_{\text{minimum}}$ and $\Omega_B = \left(\sqrt{\left|\frac{\partial^2 U}{\partial c^2}\right|/B_c}\right)_{\text{saddle}}$ are the local frequencies in the minimum c=1 and at the saddle point c=1.8 and U_B,T are the barrier height and the temperature respectively.

For the practical calculation, we assumed an excitation energy of $E^* = 80$ MeV and the relations :

$$E^* = a\,T^2 \ , \quad a = \frac{A}{10}$$

between the excitation energy and the temperature T. We assumed this temperature to be a constant along the path in order to make the comparison with Kramers results meaningful. To achieve the stationary solution as fast as possible, we decided to choose locally the following initial conditions (t=o) :

$$d_{red}(c) = \begin{cases} N \exp\left(-\frac{U(c,h_m = 0, x_m = 0)}{T}\right) d^{eq}_{red}(c) & \text{for } c < c_{saddle} = 1.8 \\ d_{red}(c_{saddle}) & \text{for } c > c_{saddle} \end{cases}$$

This means that we start locally with an equilibrium distribution $d^{eq}_{red}(c)$ weighted properly by the factor exp(- U/T). N is a normalisation factor.

In figure 2 we plotted the flux at the barrier as a function of time for a typical friction $f = \frac{\gamma}{\gamma_o} = 1$. It shows how the stationary solution is obtained. After a small oscillation the flux converges quite rapidly to its stationary value, which is almost identical to Kramers estimation.

In fig. 3 we show the decay rate (full line) in comparison with Kramers result (dashed line) as a function of $f = \gamma/\gamma_0$. The agreement between the two calculations is excellent if we consider the need to discretise the bundled propagation problem. The used discretisation induces some numerical uncertainties and could be ameliorated in further calculations. Nevertheless the most striking feature is the obtention of a nice bending over of our curve in the transitional friction regime.

Let us now treat the realistic case of the fission of ^{205}At at the rather high excitation energy of 80 MeV, which allows us to neglect shell effects and pairing. We use the shape parametrization

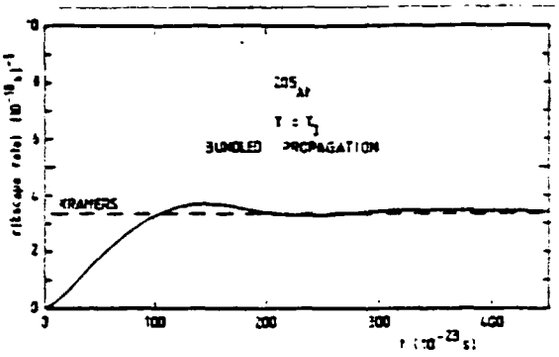

Fig. 2 : Flux at the top of the fission barrier as a function of time. The escape rate r computed in the stationary situation with a propagation on gaussian bundles (full line) is compared to the Kramers calculation for a model case $\gamma = \gamma_o$ and A = 205.

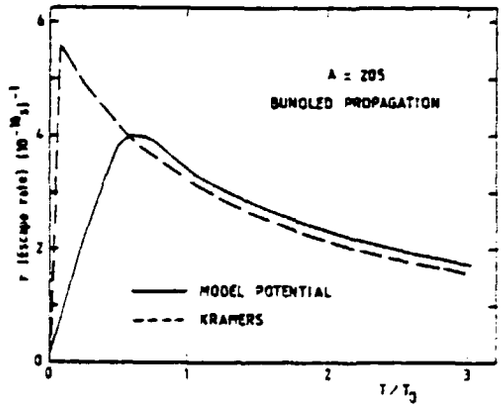

Fig. 3 : Comparison of the calculations for the escape rate with a bundled propagation and with the Kramers expressions. The escape rate r is shown as a function of the friction strength γ/γ_o, where γ_o is a reference value.

(c,h,x) of (6) with the modification of (5) for $B \equiv 2h + \frac{1}{2}(c-1) \leq 0$. The potential landscape in this functional space is shown in (6). It turns out that the path of steepest descent is not a straight line in the(c-h)plane as in our simple model case. In the practical calculation we adjust now the temperature T along the path. We assume that the total energy is conserved in the mean, viz:

$$(E^*)_c + \langle E_{coll} \rangle_c = 80 \text{ MeV}$$

where the mean collective energy $\langle E_{coll} \rangle$ is the sum of the collective kinetic and potential energy. We calculate the coordinate dependent temperature $(T)_c$ by means of :

$$(E^*)_c = \frac{A}{10} (T)_c^2 .$$

As a further modification with respect to our previous model calculation, we introduce now the generalized Einstein relation between the friction and diffusion coefficients, which, in a one dimensional case, reads :

$$D(\langle Q \rangle, T) = \gamma(\langle Q \rangle) . T^*(\langle Q \rangle, T) .$$

This relation was proven within the framework of linear response theory[13]. T^* can be interpreted as an effective temperature and is given by the formula :

$$T^* = \frac{\hbar\omega}{2} \operatorname{cotgh} \left(\frac{\hbar\omega}{2T}\right)$$

where the local frequency $\bar{\omega}(Q)$ is defined as :

$$\left[\bar{\omega}(Q)\right]^2 = \frac{\partial^2 V}{\partial Q^2}_{<Q>} / B(<Q>).$$

In the multidimensional case, the effective temperatures can be properly defined locally in the system of normal coordinates . For details we refer the reader to ref.[11].

Since the mean path out of the minimum over the barrier towards scission is of a particular interest, we show in fig. 4 how this path is affected by the coupling B_{ch} for the typical friction $f = \gamma/\gamma_o = 1$. For $B_{ch} = 0$ the system remains close to the line of steepest descent as it could be expected from purely static considerations. But after the switching on of the coupling $B_{ch} = B_c/3$ one observes a dramatic change of the mean trajectory in the region of the potential minimum. In spite of this strong deviation it comes again rather close to the line of steepest descent between saddle and scission. On the other hand the escape rate is practically independent of the coupling. For $B_{ch} = 0$ we find $\tau = 6.7 \times 10^{17}$s compared to $\tau = 6.3 \times 10^{17}$s in the case $B_{ch} = B_c/3$. One can get a remarkable decrease of the escape rate only for very strong coupling B_{ch}.

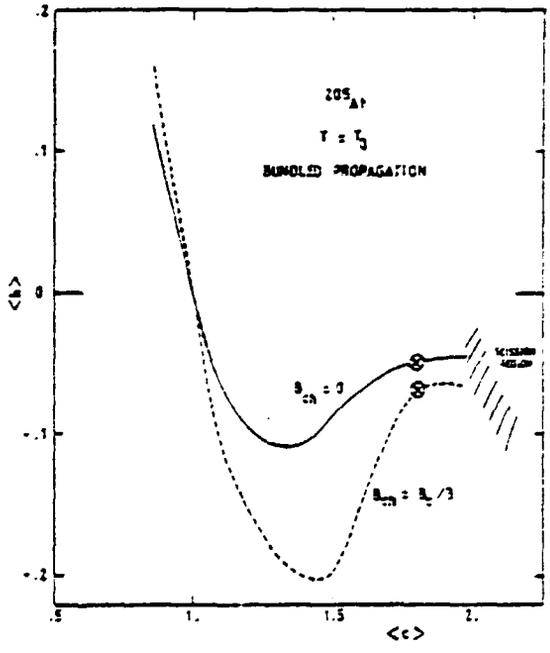

Fig. 4 : Dynamical paths for the fission of ^{205}At in the {<c>,<h>} plane. The saddle points are represented by the symbol θ for two paths obtained with coupling and without coupling terms in the transport coefficient tensors.

4. Fluctuations of the collective coordinates

The initial conditions at the saddle point have been calculated in the corresponding bundle for the precedent cases (with and without coupling). Especially for the fluctuation in mass asymmetry $\chi^{\alpha\alpha}$, in the neck coordinate χ^{hh} and in momentum along the elongation ω_{cc}, it is interesting to compare the dynamical values in the stationary situation with the bare static values obtained for a statistical equilibrium at the saddle point. As reported in Table I, the dynamical values are slightly larger for $\chi^{\alpha\alpha}$ and χ^{hh} than expected from a statistical equilibrium assumption. This fact seems to indicate that this equilibrium is not completely reached even in the stationary situation. Nevertheless, as far as the absolute values are concerned, some coordinate dependence of the transport coefficients could somewhat modify the presented results. On the other hand some smaller values of ω_{cc} are obtained in our calculation than in the equilibrium estimation. This particular result is

identical to the one obtained in the one dimensional model of ref.[2)]

Table I

Initial conditions at the saddle point for $\chi^{\alpha\alpha} = \frac{1}{2}\int d\Gamma_{red}\,(\alpha-\langle\alpha\rangle)^2 d$, $\chi^{hh} = \frac{1}{2}\int d\Gamma_{red}\,(h-\langle h\rangle)^2 d$, $\omega_{cc} = \frac{1}{2}\int d\Gamma_{red}\,(P_c - \langle P_c\rangle)^2 d$ where $d\Gamma_{red} = dP_c\,d\alpha\,dP_\alpha\,dh\,dP_h$. These values are obtained by considering for the density d ; i) a statistical distribution, ii) the stationary value dynamically computed for two different assumptions on the coupling between c and h. B_c is the inertia parameter along the c coordinate and B_{ch} the cross term between c and h in the inertia tensor.

	$\chi^{\alpha\alpha}$	χ^{hh}	$\omega_{cc}[GeV\ 10^{-23}s]^2$
Statistical equilibrium with $B_{ch}=0$	1.75×10^{-3}	3.02×10^{-3}	1.67×10^{-1}
Dynamical calculation with $B_{ch}=0$	2.50×10^{-3}	3.61×10^{-3}	1.19×10^{-1}
Statistical equilibrium with $B_{ch}=B_c/3$	1.75×10^{-3}	3.10×10^{-3}	1.84×10^{-1}
Dynamical calculation with $B_{ch}=B_c/3$	2.92×10^{-3}	5.74×10^{-3}	1.30×10^{-1}

Finally, the statistical equilibrium values are reasonable for starting a dynamical path from saddle to the scission region.

According to eq. (12) the variance in mass asymmetry was computed as a function of $\xi = \gamma/\gamma_o$. The width Γ of the mass distribution is merely :

$$\Gamma = \sigma_{AA}\sqrt{3Ln2}$$

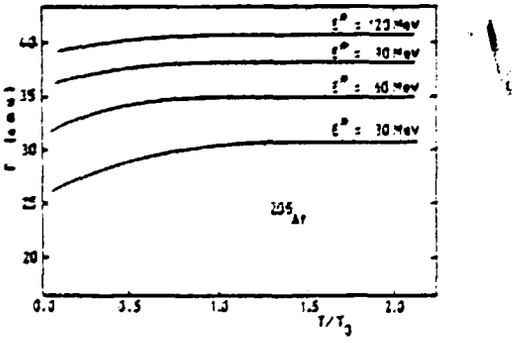

Fig. 5 : Calculated widths Γ of the mass distribution for the fission of ^{205}At. The widths are obtained for various strengths of the friction γ and for different excitation energies.

In figure 5, different curves were calculated for four excitation energies with initial conditions at the saddle chosen in a statistical equilibrium. It turns out that the final result is independent on the friction strength as far as γ exceeds roughly $\gamma_o/2$. For a comparison with the experimental

values, it must be quoted that our calculation gives Γ = 35.2 a.m.u. at an excitation energy E^* = 60 MeV and that the experimental result of ref.[12] is Γ_{exp} = 33 ± 3 a.m.u. This agreement is stimulating for further computation of macroscopic quantities by use of the transport equation (1) with a bundled propagation.

Conclusion

It was shown that the use of propagators permits to obtain a time dependent solution of the Fokker-Planck equation[2]. We have shown that the method of a bundled propagation with gaissian bundles is an excellent approximation in model cases, especially in the crucial estimation of the decay rate through a barrier. Furthermore the bundled propagation makes the solution of multidimensional Fokker Planck equationsnumerically tractable. Its application to a three-dimensional treatment of the fission process gives us a lot of information on the various steps of the dynamics. First of all the decay rate can be obtained by looking on the flux at the saddle point. Surprisingly, it appears rather insensitive to the non diagonal terms in the transport coefficient tensors. Secondly, the dynamical calculation of the initial conditions at the saddle point, starting with an equilibrium distribution in the first well, shows that the current assumption of a statistical equilibrium is reasonable in view of the small deviations that appear. Finally, first calculations concerning the width of the mass distribution for fission fragments are in remarkable agreement with the experiments. Further calculations will now be possible for estimating a lot of macroscopic quantities of interest in nuclear fission. In this spirit, microscopic transport coefficients would be required[13].

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