УДК 539.17

NON-MARKOVIAN LARGE-AMPLITUDE MOTION AND NUCLEAR FISSION

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The general problem of dissipation in macroscopic large-amplitude collective motion and its relation to the energy diffusion of the intrinsic degrees of freedom of a nucleus is studied. By applying the cranking approach to the nuclear many-body system, a set of coupled dynamical equations for the collective classical variables and the quantum mechanical occupancies of the intrinsic nuclear states is derived. Different dynamical regimes of the intrinsic nuclear motion and its consequences on time properties of the collective dissipation are discussed. The approach is applied to the descent of the nucleus from the fission barrier.

1. Introduction

Nuclear large-scale dynamics (nuclear fission, heavy ion collisions etc.) is a good probe for the investigation of the complex time evolution of finite Fermi systems. The conceptual question is here how collective modes of motion appear in a system with many degrees of freedom and how they interact with all other intrinsic modes. Nuclear collective dynamics can be studied by using the concept of macroscopic motion for a few collective degrees of freedom, which are chosen to describe gross properties of the nucleus [1 - 3]. Such a kind of approach is acceptable for a slow collective motion where the fast intrinsic degrees of freedom exert forces on the collective variables leading to a transport equation. The crucial point of such an approach is separation of the total energy of a system into the potential energy, collective kinetic energy and dissipation energy. Moreover the dissipation of collective motion implies fluctuations in the corresponding collective variables, as follows from the fluctuation-dissipation theorem [4].

Dissipation of the nuclear collective energy reveals itself, for instance, as the non-zero contribution of the internucleonic collisions to the widths of the nuclear giant multipole resonances. On the other hand, the experimental observation of the finite variance of the kinetic energy of the fission fragments manifests the fact that the fluctuations have to be also associated with the collective variables. Both the dissipation and the fluctuations can be described by the introduction of friction and random forces, related to each other by the fluctuation-dissipation theorem. In this respect, the Fokker - Planck or Langevin approaches can be used to study the nuclear large-scale dynamics. In general, basic equations of motion for the macroscopic parameters, describing complex dynamics of the many-body systems like nuclei, have a non-Markovian structure. One of the first considerations of memory (non-Markovian) effects for classical liquids can be found in Ref. [5]. For the dynamics of nuclei, memory effects have been investigated within different approaches. In this respect, one can mention the dissipative diabatic model [6], the linear response theory [3] and the fluid dynamic approach [7, 8]. In this paper, we would like to apply the non-Markovian dynamics to the study of the nuclear fission characteristics and clarify the role of the fluctuation and memory effects in the descent of the nucleus from the fission barrier to the scission point.

The plan of the paper is as follows. In Sect. 2, we derive the non-Markovian Langevin equation of motion for the nuclear shape variables starting from the collisional kinetic equation. Sect. 3 is devoted to details of the numerical determination of the saddle–to–scission time and in presence of the memory effects and the random force for the descent of the nucleus from the barrier to the scission point. Summary and conclusions are given in Sect. 4.

2. Nuclear many-body system

We assume that dynamics of nuclear many body system can be described as a coupled motion of the macroscopic collective modes and intrinsic nucleonic ones. Slow collective modes of the nuclear large-amplitude motion are treated in terms of a set of classical time-dependent variables n, while the fast intrinsic modes are described quantum mechanically through the time evolution of occupancies of nucleonic many body states.

The intrinsic dynamics can be determined through the Liouville equation for the density matrix operator $\hat{\rho}$,

$$\frac{\partial \hat{\rho}}{\partial t} + i\hat{L}\hat{\rho} = 0, \qquad (1)$$

where $\hat{L}$ is the Liouville operator defined in terms of the commutator, $\hat{L}\hat{\rho} = \left[\hat{H}, \hat{\rho}\right]/\hbar$, of the nuclear many body Hamiltonian $\hat{H}$.

Using Zwanzig's projection technique [9] and a basis of adiabatic eigenenergies E_n and eigenfunctions Ψ_n of the nuclear many body Hamiltonian [10], we can get dynamical equations for a non-diagonal part of the density matrix,

$$\rho_{nm}(t) = -i\sum_i \int_0^t ds\dot{q}(s)\frac{\exp[-i\omega_{nm}(t-s)]}{\omega_{nm}}\left[h_{i,mn}(s)\rho_{nn}(s) - h_{i,nm}(s)\rho_{mm}(s)\right], \quad (2)$$

and its diagonal part,

$$\frac{\partial\rho_{nn}(t)}{\partial t} = \frac{2}{\hbar^2}\sum_{i,j}\dot{q}_i(t)\int_0^t ds\dot{q}_j(s)\sum_{m\neq n}h_{i,nm}(t)h_{j,mn}(s)\frac{\cos[\omega_{nm}(t-s)]}{\omega_{nm}^2}\left[\rho_{mm}(s) - \rho_{nn}(s)\right]. \quad (3)$$

Here, $\omega_{nm} = (E_n - E_m)/\hbar$ and matrix elements $h_{i,nm} = \left|\partial\hat{H}/\partial q_i\right|_{nm}$ measure the coupling between the quantum nucleonic and the macroscopic collective subsystems.

To proceed further, we use a random matrix theory developed in our previous paper [10] for the case of a single collective coordinate. We omit all intermediate steps and give a basic diffusion-like equation of motion for the ensemble averaged occupancies $\bar{\rho}(E,\ t)$ of the many body states $E \equiv E_n$:

$$\Omega(E)\frac{\partial\bar{\rho}(E,\ t)}{\partial t} = \sum_{i,j}s_{ij}\dot{q}_i(t)\int_0^t ds\exp\left(-\frac{|t-s|}{\hbar/\Gamma_{ij}}\right)Y_{ij}(q[t],\ q[s])\dot{q}_j(s)\frac{\partial}{\partial E}\left[\Omega(E)\frac{\partial\bar{\rho}(E,\ s)}{\partial E}\right], \quad (4)$$

where s_{ij} and Γ_{ij} are, correspondingly, the strengths and widths of the energy distributions of the ensemble averaged coupling matrix elements $h_{i,mn}$, $Y_{ij}(q[t],\ q[s])$ are the correlation functions measuring how strong the coupling matrix elements correlate at different collective deformation parameters $q[t]$ and $q[s]$, and $\Omega(E)$ is the nuclear many body level density at excitation energy E.

2.1. Energy rate

In order to define properly dynamics of the classical collective parameters $q(t)$ within the cranking approach, one has to consider total energy of the nuclear many body system, which can be written as

$$\Sigma(t) = E_{gs}(q) + Tr\left\{\hat{H}(q[t])\hat{\rho}(t)\right\}, \quad (5)$$

Differentiating over time both sides of Eq. (6), we get

$$\frac{d\Sigma}{dt} = \sum_i \dot{q}_i\frac{\partial E_{gs}}{\partial q_i} + \sum_i \dot{q}_i\sum_{n,m}\left(\frac{\partial\hat{H}}{\partial q_i}\right)_{mn}\rho_{nm} +$$

$$+\sum_n E_n\frac{\partial\rho_{nn}}{\partial t} + \sum_i \dot{q}_i\sum_n\left(\frac{\partial\hat{H}}{\partial q_i}\right)_{nn}\rho_{nn}. \quad (6)$$

The first term in the right-hand side of Eq. (6) describes a change of the collective potential energy. The second term depends on the non–diagonal component of the density matrix $\rho_{nm}(t)$. Its time evolution is caused by the virtual transitions among adiabatic states of the nuclear many-body Hamiltonian. We believe that such a term is a microscopic source for the appearance of the collective kinetic energy:

$$\left(\frac{d\Sigma}{dt}\right)_{virt} \approx \sum_i \dot{q}_i\sum_j B_{ij}(q)\ddot{q}_j, \quad (7)$$

where B_{ij} is a collective mass parameter,

$$B_{ij} = \sum_{n,m}h_{i,nm}h_{j,mn}\omega_{nm}^{-3}[\rho_{mm} - \rho_{nn}]. \quad (8)$$

It can be easily shown that the third and fourths terms in the energy–rate expression (6) can be combined as $d(\sum_n E_n\rho_{nn})/dt$ and that is the rate of change of the intrinsic nucleonic energy $E^* = \sum_n E_n\rho_{nn}$. The energy E^* of the intrinsic excitations is defined by the real transitions between the adiabatic many body states of the system and we represent the corresponding contribution to the rate of change of the total energy of the nuclear system as follows

$$\left(\frac{d\Sigma}{dt}\right)_{real} = \frac{1}{M_q}\sum_i \dot{q}_i(t)\frac{1}{\dot{q}_i}\frac{dE^*}{dt} \quad (9)$$

where M_q is the total number of the collective degrees of freedom.

Collecting Eqs. (8) and (10), one obtains for (7),

$$\left(\frac{d\Sigma}{dt}\right)=\sum_i \dot{q}(t)F_i(q,\dot{q},t), \qquad (10)$$

where quantities F_i mean forces acting on the collective subsystem given by

$$F_i=\sum_j B_{ij}\ddot{q}_j+\frac{\partial E_{gs}}{\partial q_i}+\frac{1}{M_q}\frac{1}{\dot{q}_i}\frac{dE^*}{dt}. \qquad (11)$$

2.2. Equations of motion for the collective parameters

To get M_q equations of motion for M_q unknown collective parameters q_i, we assume that all partial contributions to the energy rate (11) are zero [1],

$$F_i=0,\ i=1,\ ...,\ M_q. \qquad (12)$$

Thus, the collective dynamics satisfy the following set of equations

$$\sum_j B_{ij}[q]\ddot{q}_j=-\frac{\partial E_{gs}}{\partial q_i}-\frac{1}{M_q}\frac{1}{\dot{q}_i}\frac{dE^*}{dt}. \qquad (13)$$

One can demonstrate that for the constant-temperature level density, $\Omega(E)=const\cdot\exp(E/T)$, where T is the temperature of the nucleus, we obtain a closed set of equations of motion for the collective parameters:

$$\sum_j B_{ij}[q]\ddot{q}_j=-\frac{\partial E_{gs}}{\partial q_i}-\sum_j\frac{s_{ij}}{T}\int_0^t dt'\exp\left(-\frac{|t-t'|}{\hbar/\Gamma_{ij}}\right)Y_{ij}(q[t],\ q[t'])\dot{q}_j(t'). \qquad (14)$$

It should be pointed out that Eq. (14) describes the ensemble averaged collective dynamics, i. e., averaged over many different random realizations of the intrinsic nucleonic subsystem. In this way, of course, we loose information about the quantum fluctuations of the intrinsic degrees of freedom of the nuclear many body system which, in principle, may be important. In order to try to take them into account somehow, we introduce a phenomenological stochastic force term, $\xi_i(t)$, into the collective equations of motion (14) and requiring that the fluctuation-dissipation theorem is hold,

$$\left\langle\xi_i(t)\xi_j(t')\right\rangle=Ts_{ij}Y_{ij}(q[t],\ q[t'])\exp\left(-\frac{|t-t'|}{\hbar/\Gamma_{ij}}\right). \qquad (15)$$

With this, the collective dynamics gets a form of the non-Markovian Langevin equations of motion

$$\sum_j B_{ij}[q]\ddot{q}_j=-\frac{\partial E_{gs}}{\partial q_i}-\sum_j\frac{s_{ij}}{T}\int_0^t dt'\exp\left(-\frac{|t-t'|}{\hbar/\Gamma_{ij}}\right)Y_{ij}(q[t],\ q[t'])\dot{q}_j(t')+\xi_i(t). \qquad (16)$$

3. Numerical calculations

Now we turn to the numerical determination of nuclear fission’s characteristics. We study the symmetric fission of highly excited heavy nuclei whose space shape may be obtained by rotation of some profile function $Y^2(z)$ around z-axis. It is considered a 2-parametric family of the Lorentz shapes [2]:

$$Y^2(z)=(z^2-\zeta_0^2)(z^2+\zeta_2^2)/Q, \qquad (17)$$

where the multiplier $Q=-\zeta_0^3(\zeta_0^2/5+\zeta_2^2)$ guarantees the conservation of the nuclear volume. Here, all quantities of the length dimension are expressed in units of the radius R_0 of the spherical equal–volume nucleus. The parameter ζ_0 in Eq. (17) defines an elongation of the figure, while ζ_2 is responsible for its neck. Thus, in the case of $\zeta_2=\infty$ we have a spheroidal shape and for $\infty<\zeta_2<0$ the neck appears.

The adiabatic collective potential energy of deformation $E_{gs}(q)$ were taken from Ref. [2]. The equations of motion (15), (16) were solved numerically with the help of the simplest Euler method with the initial conditions corresponding to the saddle-point deformation and the initial kinetic energy $E_{kin,0}=1$ MeV (initial neck velocity $\dot{\zeta}_2=0$). The numerical calculations were performed for the symmetric fission of the nucleus ^{236}U at temperature $T=2$ MeV. We define the scission line from the condition of the instability of the nuclear shape with respect to any variations of the neck radius:

$$\frac{\partial^2 E_{gs}(q)}{\partial r_{neck}^2}=0, \qquad (18)$$

where $r_{neck}=\zeta_2/\sqrt{\zeta_0(\zeta_0^2/5+\zeta_2^2)}$ is the neck radius.

We considered a time of the nuclear descent from the saddle point to the scission (18). The total number of $N = 2 \cdot 10^4$ trajectories $\varsigma_0(t), \varsigma_2(t)$, generated by the different random realizations of the random forces $\xi_i(t)$, were taken into consideration in order to define the dynamic path of the system (15), (16). To simplify the problem and clarify the role of the random force in the non-Markovian dynamics of the system, we stopped running trajectories $\varsigma_0(t), \varsigma_2(t)$ when they cross the line $r_{neck}(\zeta_0, \zeta_2) = r_{neck}^{Newt}$, where r_{neck}^{Newt} is the neck radius' value determined from the Newtonian non-Markovian dynamics (i. e., when the stochastic terms are absent in Eqs. (15), (16)).

In Fig. 1, we show the Langevin (solid line) and Newtonian (dashed line) dynamic trajectories of the neck radius $r_{neck}(t)$. Horizontal line in the figure gives the scission value of the neck radius r_{neck}^{Newt} derived from the Newtonian calculation.

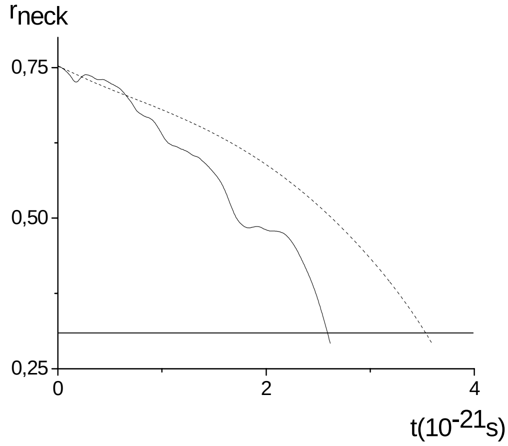

Fig. 1. Typical Langevin (solid line) and Newtonian (dashed line) trajectories of the neck radius $r_{neck}(t)$ of the system (15), (16). Horizontal line is the value of r_{neck}^{Newt} derived from the Newtonian dynamics.

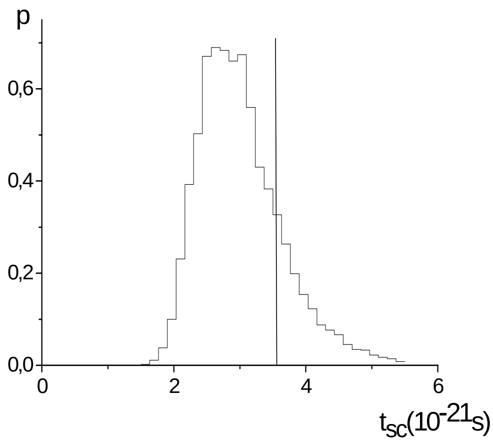

Fig. 2. Histogram of a probability density p of the descent times t_{sc} for the non-Markovian Langevin dynamics (15), (16) at the relaxation time $\tau_r \equiv \hbar/\Gamma = 2 \cdot 10^{-23} s$, when the size of memory effects is quite small. The vertical line gives the Newtonian estimation for the descent time.

A histogram of the distribution p of the saddle-to-scission times t_{sc} is given in Fig. 2. We found that the most probable and mean value of the descent time are significantly smaller than the Newtonian estimation of t_{sc} shown by a vertical line. In fact, the random force speeds up the process of descent from the fission barrier. Indeed, the action of a random force, in some sense, "shakes loose" the system giving rise to a smaller time of motion between two given points comparing to the corresponding time for the unperturbed of the system. It should be pointed out that this is hold both for Markovian Langevin dynamics (it may be demonstrated analytically for some quite simple models) and non-Markovian Langevin dynamics. The last feature is demonstrated in Fig. 3, where the mean value $\langle t_{sc} \rangle$ of the descent time is plotted versus the relaxation time τ_r for the Langevin (solid line) and Newtonian (dashed line) [11] paths of the system.

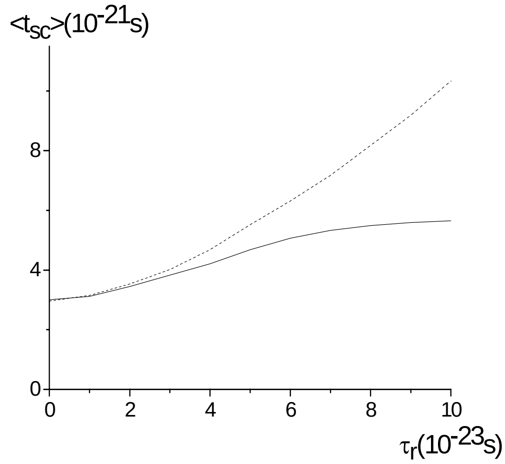

Fig. 3. The mean value of the descent time $\langle t_{sc} \rangle$ for the non-Markovian Langevin dynamics (15), (16) versus the relaxation time τ_r is shown by solid line. The Newtonian calculation of the descent time is given by the dashed line.

As seen in Fig. 3, the difference between the two non-Markovian calculations of the mean saddle-to-scission time grows with the relaxation time. This fact may be explained by the correlation properties of the random forces in the non-Markovian Langevin equations, see Eq. (15). As can be seen from Eq. (15), the increase of the relaxation time τ_r amplifies the correlation in the collective coordinates $\varsigma_0(t)$, $\varsigma_2(t)$ at two subsequent moments of time t and $t+\Delta t$. As a result, one might expect that a quite big change, occurred for the coordinates ς_0, ς_2 at time t, will give rise to a sufficiently big change for ς_0, ς_2 even at the next time step $t+\Delta t$. This tendency will be stronger as far as the relaxation time τ_r grows up. Therefore, in average the system will reach the scission faster as compared to the non-Markovian motion of the system.

4. Summary and Conclusions

Within non-Markovian Langeven approach, we have demonstrated a consistent description of nuclear large-amplitude dynamics, including the memory effects and the random force. We have averaged the intrinsic nucleonic dynamics (4) over suitably chosen statistics of the randomly distributed coupling matrix elements and the energy spacings. Owing to this procedure, we have derived the diffusion-like equation of motion for the smeared occupancies $\bar{\rho}(E,\ t)$ of the adiabatic many body states. Note that the obtained equation of motion for $\bar{\rho}(E,\ t)$ is the non-Markovian one, where the memory effects depend on the width of the randomly distributed matrix elements.

Applying the ensemble averaging procedure, we have also derived the collective mass parameter and the internal energy rate. Finally, we derive a set of coupled dynamic equations for the macroscopic variables which take into consideration the time variation of the occupancies of the intrinsic nuclear states. Following the fluctuation-dissipation theorem, we have incorporated also the relevant random force into the macroscopic equations of motion.

The main contribution to the rate of dissipation energy is due to the jump probabilities leading to a rate of dissipation which depends essentially on the total energy of the nucleus. The final result shows that a time irreversible energy exchange between the collective and internal degrees of freedom is possible when the level density increases with energy. We have applied our approach to the description of the descant of the nucleus from the fission barrier. We show that the random force accelerate significantly the process of descent from the barrier for both the Markovian and non–Markovian Langevin dynamics. We have observed that the difference between the two non–Markovian calculations (see Fig. 3) of the mean saddle-to-scission time grows with the relaxation time. This fact may be explained by the correlation properties of the random force in the non-Markovian Langevin equations.

REFERENCES

1. *Siemens P.J., Jensen A.S.* Elements of Nuclei: Many-body Physics with the Strong Interaction. - Addison and Wesley, 1987.
2. *Hasse R.W., Myers W.D.* Geometrical Relationships of Macroscopic Nuclear Physics. - Berlin, Heidelberg: Springer-Verlag, 1988.
3. *Hofmann H.* // Phys. Rep. - 1997. - Vol. 284. -P. 137.
4. *Balescu R.* Equilibrium and Nonequilibrium Statistical Mechanics. Vol. 2. - New York: Wiley, 1975.
5. *Frenkel J.* Kinetic Theory of Liquids. - Oxford: Clarendon, 1946.
6. *Ayik S., Nörenberg W.* Time-Dependent Shell-Model Theory of Dissipative Heavy-Ion Collisions // Z. Phys. - 1982. - Vol. A309. - P. 121.
7. *Kolomietz V.M.* Stochastic aspects of nuclear large amplitude motion // Phys. Rev. - 1995. - Vol. C52. - P. 697.
8. *Kolomietz V.M., Shlomo S.* Nuclear Fermi-liquid model // Phys. Rep. - 2004. - Vol. 390. - P. 133.
9. *Zwanzig R.* Ensemble Method in the Theory of Irreversibility // J. Chem. Phys. - 1960. - Vol. 33. - P. 1338.
10. *Kolomietz V.M., Åberg S., Radionov S.V.* Collective motion in a quantum diffusive environment // Phys. Rev. - 2008 - Vol. C77. - P. 04315.
11. *Kolomietz V.M., Radionov S.V., Shlomo S.* Memory effects on the descent from fission barrier // Phys. Rev. - 2001. - Vol. C64. - P. 054302.

НЕ-МАРКОВСЬКИЙ РУХ ВЕЛИКОЇ АМПЛІТУДИ ТА ПОДІЛ ЯДЕР

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Досліджується загальна проблема дисипації в макроскопічному колективному русі з великими амплітудами та її відношення до дифузії енергії внутрішніх ступіней вільності ядра. Застосовуючи cranking-наближення до ядерної багаточастинкової системи, ми одержуємо систему зв’язаних рівнянь для колективних змінних та заселеностей внутрішніх ядерних станів. Обговорюються різні динамічні режими внутрішнього ядерного руху та їх вплив на властивості дисипації в колективному русі. Підхід застосовано до опису спуску ядра з бар’єра поділу.

НЕ-МАРКОВСКОЕ ДВИЖЕНИЕ БОЛЬШОЙ АМПЛИТУДЫ И ДЕЛЕНИЕ ЯДЕР

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Исследуется общая проблема диссипации в макроскопическом коллективном движении с большими амплитудами и ее отношение к диффузии энергии внутренних степеней ядра. Применяя cranking-приближение к ядерной многочастичной системе, мы получаем систему связанных уравнений для коллективных переменных и заселенностей внутренних ядерных состояний. Обсуждаются различные динамические режимы внутреннего ядерного движения и их влияние на свойства диссипации в коллективном движении. Подход применяется к описанию спуска ядра с барьера деления.

Received 09.06.08,
revised - 23.12.08.