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STOCHASTIC RESONANCE AT DIFFUSION OVER A POTENTIAL BARRIER

The general problem of diffusive overcoming of a single-well potential barrier in the presence of a periodic time forcing is studied within the generalized Langevin approach. We found that the thermal diffusion over the barrier can be resonantly accelerated at some frequency of the periodic modulation that is inversely proportional to the mean first-passage time for the motion in the absence of the time-modulation. The resonant activation effect is rather insensitive to the correlation time of the random force term in the Langevin equation of motion.

Keywords: stochastic resonance, diffusion, potential barrier, Langevin equation, memory effects.

Introduction

Nonlinear systems with a complex dynamics may show significantly different response on an external periodic forcing than the corresponding linear systems. In this respect one can mention stochastic resonance phenomenon [1], when the response of the nonlinear system on the harmonic perturbation is resonantly activated under some optimal level of a noise. The resonant activation of the system occurs when the frequency of the modulation, ω, is close to the Kramers' escape rate, r_{Kr}, $\omega \approx r_{Kr}$, of the transitions from one potential well to another one. One can observe and measure stochastic resonance phenomenon in different physical systems like a ring laser [2], magnetic systems [3], optical bistable systems [4] and others.

In the present paper, our aim is to study thermal non-Markovian diffusion over a one-humped potential barrier in the presence of periodic time modulation.

Thermal non-Markovian diffusion over a potential barrier

We start from the generalized Langevin equation of motion for a single dimensionless coordinate $q(t)$ diffusively overcoming the potential barrier in the presence of a periodic force $F_{ext}(t) = \alpha \sin(\omega t)$ [5]:

$$M\ddot{q} = -\frac{\partial E_{pot}}{\partial q} - \int_0^t \kappa(t-t')\dot{q}(t')dt' + \zeta(t) + \alpha\sin(\omega t), \qquad (1)$$

where M is the constant mass parameter, $\kappa(t-t')$ is the memory kernel of the retarded friction force and $\zeta(t)$ is the random force. The potential energy $E_{pot}(q)$ is schematically shown in Fig. 1 and presents a single-well barrier formed by a smooth joining at $q = q'$ of the potential minimum oscillator with the inverted oscillator,

$$E_{pot}(q) = \begin{cases} \frac{1}{2}M\omega_0^2(q-q_0)^2, q < q' \\ E_b - \frac{1}{2}M\omega_1^2(q-q_1)^2, q \geq q' \end{cases}, \qquad (2)$$

where E_b is the height of the barrier (Fig. 1).

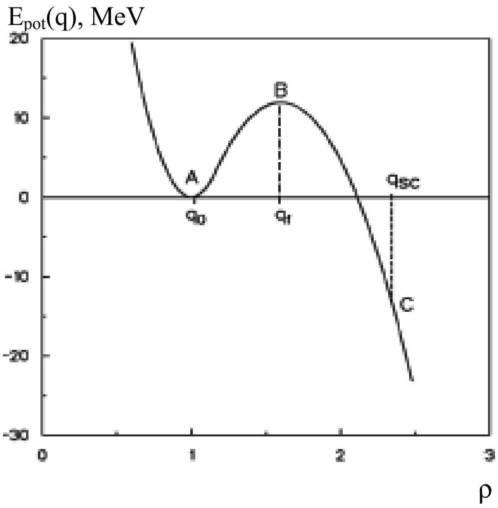

Fig. 1. A potential energy landscape defined by a smooth joining of a ground-state oscillator with an inverted saddle-point oscillator (2) with q_0 being the minimum at the point A, q_1 being the position of the top (point B) of the parabolic barrier.

A noise term $\zeta(t)$ in Eq. (1) is assumed to be Gaussian distributed with zero mean and correlation function related to the memory kernel $\kappa(t-t')$:

$$\langle \zeta(t)\zeta(t') \rangle = T\kappa(t-t'), \qquad (3)$$

where T is the temperature of the system. Below we shall assume that the memory kernel is given by

$$\kappa(t-t') = \kappa_0 \exp\left(-\frac{|t-t'|}{\tau}\right), \qquad (4)$$

where τ is a correlation time.

Unperturbed diffusion over the barrier

At the beginning, we investigated the non-Markovian diffusive dynamics for the infinitely slow ($\omega = 0$) time modulation and calculated a time-dependent escape rate $r(t)$. For that, the Langevin equation (1) was solved numerically by generating a bunch of the trajectories $\{q_i(t)\}, i = 1,..., N_0$ with the following initial conditions:

$$q_i(0) = q_0, \quad \langle \dot{q}_i(0) \rangle = 0, \quad \langle \dot{q}_i^2(0) \rangle = T / M \ , \quad (5)$$

where N_0 is a total number of the trajectories involved in the calculations.

The escape rate over the barrier was defined by

$$r(t) = -\frac{1}{P(t)} \frac{dP(t)}{dt}, \quad (6)$$

where $P(t)$ is the survival probability, i.e., probability of finding the system on the left from the top of the barrier till the time t:

$$P(t) = \frac{N(t)}{N_0}. \quad (7)$$

Here, $N(t)$ is a number of the trajectories which do not reach the top of the barrier before the time t. In the numerical calculations, all quantities of the dimension of energy is measured in units of the temperature T of the system, quantities of the dimension of time are taken in units of $\sqrt{M / T}$. For the system's parameters we adopted the following values:

$$q_0 = 1, \quad q' = 1.2, \quad q_1 = 1.6, \quad \omega_0 = 6.75,$$

$$\omega_1 = 9.59, \quad E_b = 5.15, \quad \kappa_0 = 1920, \quad (8)$$

which are typical for diffusion-like studies of fission of highly excited atomic nuclei, see Ref. [6].

In Fig. 2, the typical time behavior of the escape rate $r(t)$ is plotted for two values of the correlation time τ: $\tau = 0.005$ (when the memory effects in the diffusive dynamics Eqs. (1) - (6) are quite weak) and $\tau = 0.025$ (when the memory effects are fairly strong), see [6].

It is seen from Fig. 2 that initially the escape is affected by transient effects, when the survival probability $P(t)$ deviates strongly from the exponential form. With time, the escape process becomes more and more stationary giving rise to the corresponding saturation of the rate $r(t)$ of Eq. (6) establishing of a quasistationary probability flow over the barrier. Qualitatively, one can describe typical time evolution of the escape rate as

$$r(t) = r_0 \left(1 - \exp[-t / t_{tran}]\right). \quad (9)$$

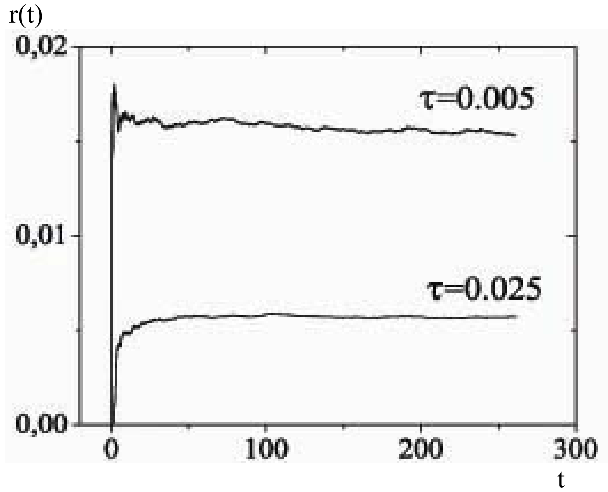

Fig. 2. The time dependence of the escape rate $r(t)$ (see Eq. (6)) for the non-Markovian diffusion dynamics Eqs. (1) - (6) calculated for two values of the correlation time τ: $\tau = 0.005$ (when the memory effects in the diffusive dynamics are quite weak) and $\tau = 0.025$ (when the memory effects are fairly strong), see [6].

In both cases a duration of the transient time, t_{tran}, is almost the same ($t_{tran} \approx 50$) for quite weak and fairly large memory effects in the diffusion process. However, a saturation value, r_0, of the escape rate is significantly different. It is because of the memory effect for the large values of the correlation time τ.

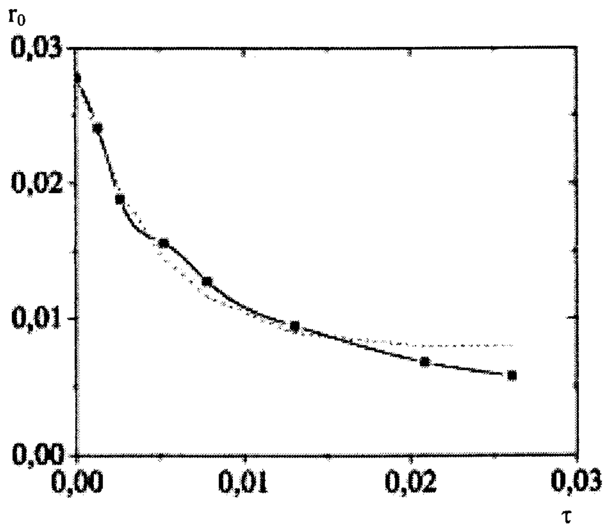

Fig. 3. The saturation value r_0 of the escape rate (see Eq. (9)) vs the correlation time τ, measuring the strength of the memory effects in the non-Markovian diffusion dynamics (see Eqs. (1) - (6)). The dotted line represents the Kramers' result of Eq. (10) for the escape rate calculated with the τ-dependent friction coefficient of Eq. (11).

In Fig. 3, we showed how the value r_0 of Eq. (9) depends on the strength of the memory effects in the diffusive dynamics Eq. (1). Dotted line in Fig. 3 represents the famous Kramers' result for the escape rate [6]

$$r_{Kr} = \frac{\omega_0}{2\pi}\left(\sqrt{\left(\frac{\gamma}{2M\omega_1}\right)^2 + 1} - \frac{\gamma}{2M\omega_1}\right)\exp\left(-\frac{E_b}{T}\right), \quad (10)$$

where the friction coefficient γ is assumed to be τ-dependent [5]

$$\gamma(\tau) = \frac{\kappa_0 \tau}{1 + (\kappa_0 / M)\tau^2} . \quad (11)$$

In paper [5], the friction coefficient of Eq. (11) is used within the Fermi-liquid approach to the nuclear collective motion with τ being the relaxation time of the collective excitations. There, $\gamma(\tau)$ is taken as an interpolation formula for the τ-dependent friction coefficient between the first-sound regime (i. e., the regime of quite frequent collisions between nucleons, $\sqrt{\kappa_0 / M}\tau << 1$, when $\gamma(\tau) \propto \tau$) and the zero-sound regime (i. e., the regime of fairly rare collisions between nucleons, $\sqrt{\kappa_0 / M}\tau >> 1$, when $\gamma(\tau) \propto 1/\tau$).

We see that the memory effects significantly suppress the value of the escape rate in the saturation regime of probability flow over the potential barrier. Initially (i. e., at relatively small values of the correlation time τ) the suppression is mainly caused by the growing role of the usual friction in the non-Markovian diffusion motion Eqs. (1) - (6). As is followed from Fig. 3, in this case the escape rate at saturation r_0 (9) may be quite well approximated by the Kramers' formula, see Eq. (10). On the other hand, at relatively large correlation times τ, the effect of the friction on the diffusion over the barrier is negligibly weak and the escape rate's suppression appears exclusively due to the additional conservative force, see Ref. [6]. As a result, the stationary value of the escape rate deviates substantially from the Kramers' escape rate Eq. (10) at the fairly strong memory effects in the diffusive motion across the barrier. Note also that, as shown in [8] and [9], the characteristics of the escape process depend much on the shapes of the potential barrier. Thus, for more complicated shapes (than the parabolic one shown in Fig. 1) of the potential energy $E_{pot}(q)$, the Kramers' model [7] cannot be applied.

Periodic perturbation effect on the thermal non-Markovian diffusion over the barrier

Now we will study the dynamics over the barrier Eqs. (1) - (6) in the presence of the external harmonic force. We will assume that the amplitude α of the force $\alpha\sin(\omega t)$ in Eq. (1) is so small ($\alpha = 0.05$) that still the reaching the top of the barrier is caused exclusively by diffusive nature of the dynamics. In Fig. 4, we calculated the typical dependencies of the mean first-passage time τ_{mfpt} (as a mean time of the first crossing of the top of the barrier) on the frequency ω of the external harmonic force. The calculations were performed for the weak, $\tau = 0.05$ (*lower curve* in Fig. 4) and strong, $\tau = 0.025$ (*upper curve* in Fig. 4) memory effects in the non-Markovian diffusive motion over the barrier.

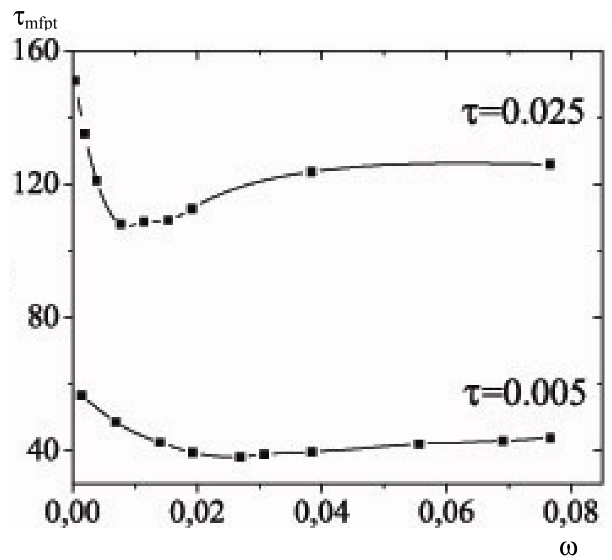

Fig. 4. The mean first-passage time τ_{mfpt} of the non-Markovian diffusion motion of Eqs. (1) - (6) is given as a function of the frequency ω of the harmonic time perturbation at two values of the correlation time $\tau = 0.05$ (*lower curve*) and $\tau = 0.025$ (*upper curve*).

In both cases the mean first-passage time τ_{mfpt} non-monotonically depends on the frequency of the perturbation that is character for the stochastic resonance phenomenon observed in a number of different physical systems. From Fig. 4 one can conclude that diffusion over the potential barrier in the presence of the harmonic time perturbation is maximally accelerated at some definite so to say resonant frequency ω_{res} of the perturbation,

$$\omega_{res} \approx \frac{1.5}{\tau_{mfpt}(\omega = 0)} . \quad (12)$$

In fact, the quantity $\tau_{mfpt}(\omega = 0)$ presents the characteristic time scale for the diffusion dynamics of Eq. (1). In the case of adiabatically slow time variations of the harmonic force, $\omega << \omega_{res}$, one can approximately use $\alpha\sin(\omega t) \approx \alpha\omega t$ and the diffusion over the barrier is slightly accelerated. As a result, the mean first-passage time $\tau_{mfpt}(\omega)$ is smaller than the corresponding unperturbed value $\tau_{mfpt}(\omega = 0)$. The same feature is also observed at the fairly large modulation's frequencies, when $\omega >> \omega_{res}$. In this case the harmonic perturbation $\alpha\sin(\omega t)$ may be treated as a random noise term with the zero mean value and variance α^2. Such a new stochastic term will lead to additional acceleration of the diffusion over the barrier.

Conclusions

We have investigated how model dynamics of the non-Markovian diffusion over the single-well parabolic barrier is affected by the external periodic time modulation. We have calculated both the mean first-passage time τ_{mfpt} and the escape rate $r(t)$ over the barrier. These two quantities have been found to be sensitive to the relative strength of memory effects in the diffusive dynamics Eqs. (1) - (6), measured by the correlation time τ. Having calculated the mean first-passage time τ_{mfpt} for different values of the frequency ω of the modulation, we have found that the sinusoidal perturbation accelerates the diffusion over the barrier, see Fig. 4. The maximal (resonant) acceleration is achieved at the $\omega = \omega_{res}$, where ω_{res} is inversely proportional to the mean first-passage time in the absence of the modulation, see Eq. (12). We have seen that a value of the resonant activation over the barrier $\tau_{mfpt}(\omega_{res}) / \tau_{mfpt}(\omega = 0)$ remains practically the same for the quite weak as well as for the fairly strong memory effects in the diffusive dynamics.

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СТОХАСТИЧНИЙ РЕЗОНАНС ПРИ ДИФУЗІЇ ЧЕРЕЗ ПОТЕНЦІАЛЬНИЙ БАР’ЄР

У рамках узагальненого ланжевенівського підходу досліджується загальна проблема дифузійного проходження через одноямний потенціальний бар’єр у присутності періодичного часового збурення. Знайдено, що теплова дифузія через бар’єр може бути резонансно-прискорена при деякій частоті періодичного збурення, яка обернено пропорційна до середнього часу першого перетину вершини потенціального бар’єра при русі без збурення. Установлено, що явище резонансної активації дифузії слабко залежить від часу кореляції випадкової сили у ланжевенівському рівнянні руху.

Ключові слова: стохастичний резонанс, дифузія, потенціальний бар’єр, рівняння Ланжевена, ефекти пам’яті.

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СТОХАСТИЧЕСКИЙ РЕЗОНАНС ПРИ ДИФФУЗИИ ЧЕРЕЗ ПОТЕНЦИАЛЬНЫЙ БАРЬЕР

В рамках обобщенного ланжевеновского подхода исследуется общая проблема диффузионного прохождения через одноямный потенциальный барьер в присутствии периодического временного возмущения. Найдено, что тепловая диффузия через барьер может быть резонансно-ускорена при некоторой частоте периодического возмущения, которая обратно пропорциональна среднему времени первого пересечения вершины барьера при движении без возмущения. Установлено, что явление резонансной активации диффузии слабо зависит от времени корреляции случайной силы в ланжевеновском уравнении движения.

Ключевые слова: стохастический резонанс, диффузия, потенциальный барьер, уравнение Ланжевена, эффекты памяти.

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