Thermal escape from a trap over the parabolic barrier: Langevin type approach to energy diffusion regime

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Abstract. Thermally activated escape from a metastable state is a useful tool to account for some features of the micro/nano-motors or superconducting nanowires. In the present work, we consider the case of week friction (action diffusion regime) which corresponds to the latter example. To describe the thermal decay, we apply two approaches both based on the Langevin type equations: the action diffusion (approximate) and the phase space diffusion (exact). For the first time, the quasistationary decay rates obtained numerically for the parabolic barrier from these two approaches are compared quantitatively with each other as well as with the analytical formula.

1. Introduction

In his pioneering work [1] Kramers indicated two regimes of the thermal decay of a metastable state (i.e. of the escape of a Brownian particle from a potential pocket or trap). Nowadays these regimes are called the spatial and energy diffusion regimes [2,3]. In the present work, we concentrate on the latter which corresponds to weak dissipation. Presently the thermal decay in the energy diffusion regime is an actual problem since it might be applied in particular to describe some features of superconduction in nanowires [4–6].

Quantitatively, the energy diffusion regime corresponds to the following inequality

\[ \varphi = \frac{\eta \tau_c}{2 \pi m} < 1. \]  \hspace{1cm} (1)

Here \( \eta \) and \( m \) denote the friction and inertia parameters, respectively; \( \tau_c \) is the period of oscillations of the particle near the bottom of the trap. We call \( \varphi \) the damping parameter henceforth.

To describe the process in the energy diffusion regime, Kramers in [1] derived an approximate equation

\[ \frac{\partial g}{\partial t} = \beta \frac{\partial}{\partial I} \left(I g + \Theta I \frac{\partial g}{\partial E} \right) \]  \hspace{1cm} (2)

Here \( g(I, t) \) is the probability density; \( \beta \) is the damping coefficient (\( \beta = \eta m^{-1} \)); \( \Theta \) is the average thermal energy; \( E \) stands for the particle energy. The action \( I(E) \) reads
\[ I(E) = 2 \int_{q_L}^{q_R} \left[ 2m(E - U(q)) \right]^{1/2} dq. \]

Here \( q \) denotes the coordinate of the Brownian particle; \( U(q) \) is the potential energy; \( q_L \) (\( q_R \)) corresponds to the left (right) turning point.

Equation (2) is a diffusion equation in the “space” whose coordinate is either energy or action; therefore, the corresponding approach is called the energy (or action) diffusion approach (ID approach). The approximate equation (2) has been obtained from the more general (and more precise) Fokker-Planck equation for the probability density in the phase space \( P(q,p,t) \) [7]:

\[ \frac{\partial P}{\partial t} = -\frac{\partial}{\partial q} \left[ \frac{p}{m} P \right] + \frac{\partial}{\partial p} \left[ \left( \eta + \frac{dU}{dq} + \eta \frac{\partial}{\partial p} \right) P \right]. \]  

(4)

The applicability of Eq. (4) is not restricted with respect to the value of the damping parameter. It is natural to call the approach based on Eq. (4) the phase space diffusion (PSD) approach.

In the problem of the decay of a metastable state (the Kramers problem), one is interested in the quasistationary decay rate resulting, e.g. from Eq. (2) or from Eq. (4). From Eq. (2) Kramers obtained an approximate analytical formula for the quasistationary rate

\[ R_K = \frac{2\pi \varphi G}{\tau_c} \exp(-G). \]

(5)

We call \( G = U_b \theta^{-1} \) the governing parameter henceforth; \( U_b \) is the height of the barrier restricting the trap.

Thus, the following questions arise: (i) at what values of \( \varphi \) and to what extent the approximate quasistationary decay rate resulting from the action diffusion approach, \( R_{DI} \), deviates from the exact rate resulting from the phase space approach, \( R_{DPS} \), and (ii) what is the amount of agreement between \( R_{DI} \) and \( R_K \). This is the goal of the present work to provide the quantitative answers to these questions for the case of the parabolic barrier. For the cases of medium [8] and large [9,10] friction, these questions were studied earlier, for the energy diffusion regime they are addressed for the first time.

2. Model

Basing on our previous expertise [9,11,12], we model the decay process by means of the Langevin equations. For the exact phase space approach, these equations are equivalent to Eq. (4); they can be found in many papers (see e.g. [12–14]). For the energy diffusion approach, there is a challenge because both \( E \) and \( I(E) \) present in Eq. (2) explicitly. After some transformations accounting for

\[ \frac{d^2 I}{dEdI} = 0 \]

we obtain the following equation

\[ \frac{\partial g}{\partial t} = \beta \frac{\partial}{\partial I} \left( I g - I' \theta g + \theta \frac{\partial (g l'I')}{\partial l} \right). \]

(7)

Here \( l' = dI/dE \), moreover this derivative must be expressed as a function of \( l \). The corresponding Langevin equation for the stochastic variable \( l \) in the numerical form (the Euler-Maruyama method [15]) reads

\[ I_{n+1} = I_n - \beta(l_n - \theta l'_n) \tau + \sqrt{\beta \theta l'_n l_n \tau} b_n. \]

(8)

Here \( l_n \) \( (l_{n+1}) \) is the action of the Brownian particle at the time moment \( t_n \) \( (t_{n+1}) \), \( \tau \) is the time step of the simulations, \( b_n \) is the normally distributed random number with zero average and variance 2.

We perform numerical modeling of Eq. (8) with \( I(E) \) corresponding to the potential represented by two parabolas of the same stiffness \( C_0 = 4U_b/(q_b - q_c)^2 \) smoothly jointed at \( q_m = (q_b + q_c)/2 \).
(“parabolic potential”). The potential of this shape is employed in many papers (see, e.g. [12,16,17]). For the quasistationary and barrier coordinates, we use \( q_c = 1.00, q_b = 1.60 \). The corresponding potential as well as the action and its derivative are shown in Fig. 1. For the harmonic oscillator the action is proportional to the energy: \( I = \tau_c E \). This analytical dependence is plotted in Fig. 1b by the dashed line. It appears that the action for the parabolic potential (the curve with symbols in Fig. 1b) behaves almost in the same way; slight deviation is seen only near the barrier. But in fact, the two actions start to be different at \( I = 0.5U_b \) as it is seen in Fig. 1c.

![Figure 1](image)

**Figure 1.** The reduced (dimensionless) values of the potential energy as a function of the coordinate (panel a), the action as a function of the reduced energy (panel b) and its derivative as a function of the reduced action (panel c).

The initial value of the action is \( I_0 = 0.01\tau_c \). The modeling lasts until either the time lapse \( t_D \) is expired or the action exceeds the value \( I(U_b) \) which plays a role of the absorptive border.

The modeling results in \( N_{tot} \) trajectories which enable us to find the time-dependent decay rate
\[ R_a(t) = \frac{1}{N_{\text{tot}} - N_{\text{at}}} \frac{\Delta N_{\text{at}}}{\Delta t} \]  

(9)

Here \( N_{\text{at}} \) is the number of trajectories which have reached the absorptive border by the time moment \( t \); \( \Delta N_{\text{at}} \) is the number of trajectories which have reached this border during the time interval \( \Delta t \). Examples of the time-dependent rates can be found in many papers (see, e.g. [12, 13, 16]). We show in Fig. 2 only one typical example with the aim to explain the automated algorithm of finding a valid value of \( R_D \) with high accuracy.

![Graph](image)

**Figure 2.** Typical time-dependent rates (wriggling lines) and their quasistationary values (horizontal lines) for two ways of modeling. Oscillating line with circles (squares) corresponds to the ID (PSD) approach. \( G = 3 \), the PSD modeling has been performed for \( \varphi = 2.55 \times 10^{-3} \).

We see in Fig. 2 that after some relaxation time, the dynamical rate reaches a quasistationary value \( R_D \). Note that the duration of the relaxation stage strongly depends upon \( \varphi \) and \( G \). In order to find \( R_D \) we use the following algorithm:

1) The simulation time lapse \( t_D \) is always divided into the very same number of bins \( i_D \) (usually 100) irrespectively of \( \varphi \) and \( G \). Thus, the bin width varies significantly with \( \varphi \) and \( G \).

2) The rate \( R_{\text{at}}(t_j) \) is calculated according to Eq. (9).

3) The limit for the relative error \( \tilde{\varepsilon} = 0.01 \) and service integer number \( k = 0 \) are established.

4) Three couples of values for \( R_{D_i} \) and \( \Delta R_{D_i} \) for \( i = k; i_1 = k + 1; i_2 = k + 2 \) are calculated within the interval \( \Delta t_{D_i} = 0.1 t_D (1 + 0.1i) \) located in the very end of the simulation time lapse \( t_D \) according to the standard statistical formulas:

\[ R_{D_i} = \frac{1}{N_{t_{D_i}}} \sum_{\text{within } \Delta t_{D_i}} R_a(t_j), \]  

(10)

\[ \Delta R_{D_i} = \frac{1}{\sqrt{N_{t_{D_i}}}} \left[ \frac{1}{N_{t_{D_i}} - 1} \sum_{\text{within } \Delta t_{D_i}} (R_a(t_j) - R_{D_i})^2 \right]^{1/2}, \]  

(11)

where \( N_{t_{D_i}} \) denotes the number of values \( R_a(t_j) \) appeared in interval \( \Delta t_{D_i} \).
5) Next, \( R_D = (R_{DI2} + R_{DI0})/2, \Delta R_D = (\Delta R_{DI2} + \Delta R_{DI0})/2 \) are evaluated.

6) Provided \(|R_{DI2} - R_{DI0}| < \Delta R_D \) and \( \Delta R_D < \bar{\varepsilon} R_D \), the process of finding \( R_D \) is considered to terminate successfully.

7) If conditions 6 are not obeyed, \( k \) is increased by 1, and stages 4-6 are repeated. The maximum allowed value of \( k = 0.8 t_D \).

8) If \( k = 0.8 i_D \) is achieved but conditions 6 are not yet obeyed, \( \bar{\varepsilon} \) is increased by 0.001, and stages 4-7 are repeated.

9) If the value \( \bar{\varepsilon} > 0.02 \) is reached, the process of finding \( R_D \) is considered to terminate unsuccessfully; one needs to repeat the dynamical modeling with either a larger \( t_D \) at the same \( N_{\text{tot}} \) or a larger \( N_{\text{tot}} \) at the same \( t_D \).

The structure of Eq. (7) implies that its solutions are self-similar, and provided one finds the decay rate at one value of the damping coefficient, the rate for any other value can be found from

\[
\frac{R_{a1}(t \beta_1)}{\beta_1} = \frac{R_{a2}(t \beta_2)}{\beta_2} \tag{12}
\]

while inequality (1) is fulfilled. Moreover, the computer modeling of the ID approach is much faster than the PSD approach. These two points make the ID approach very attractive from the computer time point of view. However, one should keep in mind that the PSD approach is exact within the statistical errors.

3. Results
In Fig. 3 we compare the quasistationary rates obtained within the framework of the ID approach by means of the approximate Kramers formula (5) and resulting from the numerical modeling based on Eqs. (8)-(10), \( R_{DI} \). As far as we are aware this comparison is performed for the first time. Because the rates depend upon the governing parameter \( G \) exponentially, we present their ratio (see the figure caption). We see that the Kramers rate disagrees with more exact dynamical rate \( R_{DI} \) in the whole range of \( G \) except probably the largest value of the governing parameter. At \( G \leq 2 \) the dynamical rate exceeds \( R_K \) because the quasistationary distribution of particles in the trap has not enough time to be established. The reason why at \( G > 2 \) the dynamical rate is smaller than \( R_K \) is less clear. Note that in the opposite limiting case with respect to the dissipation, the overdamped motion, the agreement between the corresponding dynamical and approximate Kramers rates for the same potential energy profile is much better [9].

![Figure 3](image-url)

Figure 3. The dependence of ratio \( r_{IK} = R_{DI}/R_K \) upon the governing parameter \( G \).
We go over now to the quantitative comparison between the quasistationary rates $R_{DI}$ and $R_{DPS}$ resulting from ID and PSD approaches, respectively. For this aim the ratio

$$r_{PSI} = \frac{R_{DPS} \varphi_I}{R_{DI} \varphi_{PS}}$$  \hspace{1cm} (13)

is plotted in Fig. 4.

The quantities $\varphi_I$ and $\varphi_{PS}$ are the values of the damping parameter with which the modeling according to the ID and PSD approaches has been executed, respectively. One observes the best agreement between two approaches at the smallest values of the damping parameter as is expected. However, the ratio at the fixed value of $\varphi$ depends significantly upon $G$: the level of agreement between $R_{DI}$ and $R_{DPS}$ becomes worse at large values of the governing parameter. This dependence is a novel and unexpected result of our study.

Figure 4. The dependence of ratio $r_{PSI}$ upon the governing parameter $G$ for several values of damping parameter indicated in the figure.

4. Conclusions

We have performed computer modeling of the thermal decay of a metastable state in the domain of the friction strength corresponding to the action diffusion regime. This has been made using two approaches. The first one (the action or energy diffusion approach, ID) is the approximation neglecting the dissipation in one bounce of the Brownian particle in the potential pocket. The Langevin type computer modeling using this approach has been performed for the first time. This modeling is fast and the equation is self-similar with respect to the damping coefficient.

The second one (the phase space diffusion approach, PSD) does not make the approximation inherent to the ID approach; the random walking is simulated in the phase space. Computer modeling within this approach is much slower and the equations are not self-similar.

Comparing these approaches, we have estimated the accuracy and errors of the ID approach. In particular, we have shown that the accuracy of the ID approach depends not only upon the dissipation strength (which is to be expected) but also upon the value of the governing parameter. We hope, that our results will help to other scholars, on one hand, avoiding inaccuracies related with the application of the faster ID approach and, on the other hand, saving computer resources when it is applicable.
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