Thermal Decay of a Metastable State: the Quasistationary Rate and the Mean Lifetime

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Abstract. In many branches of science, the quasistationary decay rate often is considered to be identical to the inverse mean lifetime of a Brownian particle in a metastable state. We check this presumption numerically modeling the process using the stochastic differential equations (Langevin equations). Our results define the borders of the applicability of this presumption: the ratio of the potential barrier height to the thermal energy is larger than 4. For the smaller values of this ratio, the difference between the mean lifetime and the inverse quasistationary rate achieves several tens percent. This difference depends noticeably upon the strength of dissipation.

1. Introduction

For the machines of the everyday life, thermal fluctuations hardly can be detected. Yet presently the work of nanomachines is studied experimentally [1–3]. At this scale, thermal fluctuations play a significant role. With respect to the problem of thermal decay of a metastable state, these are exactly the thermal fluctuations that govern the whole process.

The decay of the metastable state is characterized mainly by two dimensionless parameters: the governing parameter \( G = \frac{U_b}{\theta} \) and the damping parameter \( \varphi = \frac{\beta}{\omega} \). Here \( U_b \) denotes the potential barrier height (activation energy), \( \theta \) stands for the thermal energy proportional to the temperature of the thermostat, \( \beta \) is the damping coefficient, and \( \omega \) represents the frequency of oscillations at the potential minimum (see figure 1 below).

The mean lifetime of a Brownian particle before its escape is the principal characteristic of the process. In the literature, often the Kramers (or quasistationary) rate [4] is considered to be identical to the inverse mean lifetime of the Brownian particle in the metastable state [5–8]. In particular, some debates on this point appeared in the literature with respect to the nuclear fission problem [9–11]. The relationship between the approximate analytical Kramers rate and the exact numerical rate was studied in several articles [12,13].

The goal of the present contribution is to study quantitatively to what extent the numerical quasistationary decay rate \( R_{dqsa} \) is close to (or different from) the inverse mean lifetime of the metastable state, \( \tau_{am}^{-1} \), for different values of \( G \) and \( \varphi \).

2. The model

The random walk of a Brownian particle is modeled in the literature using different approaches. For the medium values of \( \varphi \) (around 1) often the Langevin equations are used, sometimes accounting for several degrees of freedom [13–17]. At extremely small values of the damping parameter, Kramers obtained an approximate formula for the quasistationary decay rate using an equation describing the diffusion along the action (or energy) variable [4]. This is called the energy diffusion regime. For
medium values of the damping parameter, the process is described either by the Fokker-Planck equation or by the stochastic differential (Langevin) equations considering the evolution of both the coordinate and the conjugate momentum. This regime can be called the phase space diffusion regime. At very large \( \varphi \) the diffusion process usually is described in the configuration space whereas the momentum is supposed to relax quickly. This is called the overdamped regime and the process is described by the Smoluchowski equation. Both of the limiting approaches used for the energy diffusion and overdamped regimes are approximate.

In the present work, we use the very same Langevin equations for the one-dimensional motion at all values of the damping parameter \( 10^{-3} < \varphi < 15 \). The motion is described by the dimensionless coordinate \( q \) and the conjugate momentum \( p \). In the discrete form, the Langevin equations read:

\[
p^{(n+1)} = p^{(n)}(1 - \eta m^{-1}) + K \tau + g b^{(n)} \sqrt{\tau},
\]

\[
q^{(n+1)} = q^{(n)} + \left( p^{(n)} + p^{(n+1)} \right) \tau / (2m).
\]

The superscripts correspond to two consequent moments of time separated by the time step of computer modeling \( \tau \). The random numbers \( b \) (last term in equation (1)) have a Gaussian distribution with zero average and variance equal to 2. In equation (1), \( m \) and \( \eta \) are the inertia and friction parameters, respectively; \( K = -dU/dq \) is the driving force; \( g = \langle \theta \eta \rangle^{1/2} \) stands for the amplitude of the random force. The potential energy \( U(q) \) is shown in figure 1. It is represented by two parabolas of the same stiffness smoothly jointed at \( q_m \) which is positioned in the middle between the quasistationary point \( q_c = 1.0 \) and the barrier point \( q_b = 1.6 \). All the trajectories begin at \( q_c \) with zero momentum.

After performing computer modeling, we have \( N_{tot} \) trajectories. All of them are terminated not later than at the time moment \( t_D \). Some of the trajectories reach the absorptive border \( q_a = 2.2 \) before \( t_D \). The algorithms for calculating the time-dependent decay rate \( R_{at}(t) \) as well as the quasistationary decay rate \( R_{dqs} \) are described in detail in [13,15].

The mean lifetime \( \tau_{am} \) is calculated according to the routine proposed in [18]:

\[
\tau_{am} = N_{tot}^{-1} \left[ \sum_{i=1}^{N_{dD}} \tau_{at} + (N_{tot} - N_{dD}) \left( t_D + R_{dqs}^{-1} \right) \right].
\]

Here the sum runs over all the trajectories \( N_{dD} \) that escape in the dynamical regime (before \( t_D \)). The rest of the trajectories, \( N_{tot} - N_{dD} \), escapes in the quasistationary regime with the average time \( t_D + R_{dqs}^{-1} \).

![Figure 1. The potential energy \( U(q) \) used in the present modelling.](image)

3. Results
The time-dependent decay rates \( R_{at}(t) \) are the key quantities of our study; therefore, we show those in figures 2 and 3. Although in these figures only 12 rates are shown, altogether there are 66 rates involved in the analysis. In each panel together with \( R_{at}(t) \) (oscillating curve with symbols), we
Figure 2. The typical decay rates as functions of time for two values of the governing parameter ($G = 0.7$ and 1.5) and three values of the damping parameter indicated in the figure.

present the resulting quasistationary rate $R_{dqs}$ (horizontal line). One sees in the figures that the value of $R_{dqs}$ covers 4 orders of magnitude: from 30 (figure 2b) down to 0.03 (figure 3f). The statistical errors of $R_{dqs}$ in all cases are smaller than 2%. Some of the calculations (e.g. like in figure 3f) requires extremely large computer resources. It is crucial for our analysis to make sure that $R_{at}(t)$ reaches the saturation (see figures 3c and 3f), i.e. that the value of $t_D$ is chosen long enough. This is controlled by a service computer program which was specially developed for this purpose. On the other hand, for small values of the governing parameter, sometimes almost all trajectories reach the absorption border during $t_D$ resulting in huge oscillations of $R_{at}(t)$. Again, the service program allows processing the same array of trajectories with a smaller value of $t_D$ getting rid of this shortcoming.

The values of $\tau_{am}$ (symbols) and $R_{dqs}^{-1}$ (lines) obtained from the numerical modeling are presented in figures 4a and 4b. The lines and corresponding symbols are rather close. However, the mean lifetimes and inverse rates vary strongly with the values of the governing and damping parameters. Therefore, it is convenient to analyze their interrelation using the relative fractional difference

$$\xi_{RT} = 1 - \tau_{am}R_{dqs}.$$
This quantity is presented in figure 4c as a function of the governing parameter for 6 values of $\varphi$. First, this figure implies that $\tau_{am}$ is always larger than $R_{dqs}^{-1}$. This is to be expected due to the transient stage seen in figures 2 and 3. Then one sees that for large values of $G$ it is correct to identify $\tau_{am}$ and $R_{dqs}^{-1}$ within the framework of 5% for all values of the damping parameter. As the governing parameter decreases, the $\xi_{R_T}(G)$-dependence begins to feel the value of $\varphi$. The curves are clearly split into two groups corresponding to the spatial diffusion regime ($\varphi = 15$ and 2.6) and the energy diffusion regime ($\varphi = 0.051, 0.0051,$ and $0.0015$). Inside each group, the values of $\xi_{R_T}$ for the same $G$ are indistinguishable within the statistical errors. This finding can be useful for avoiding superfluous and rather computer resources consuming calculations.

The curve corresponding to $\varphi = 0.51$ does not belong to any group. Indeed, this value of $\varphi$ represents a dividing range between the two regimes. It is interesting to see that this particular curve is definitely closer to the spatial diffusion regime at larger values of $G$ and gets closer to the energy diffusion regime at smaller values of the governing parameter. It is known that the two regimes are physically different with respect to the energy dissipation during one bounce of the Brownian particle in the potential well. Therefore, we interpret the $\xi_{R_T}(G)$-behaviour at $\varphi = 0.51$ in the following way. The larger value of the governing parameter suggests a higher barrier which forces the particle to make many bounces before the escape. Thus, relatively weak dissipation has enough time to influence the escape rate. At small values of $G$ (low barrier), the particle escapes making just several bounces, therefore, the weak dissipation has no time for affecting the rate.

In general, it is seen from figure 4c that, for the energy diffusion regime, one should identify $\tau_{am}$ and $R_{dqs}^{-1}$ with care, especially for comparatively small values of the governing parameter.
**Figure 4.** (a) and (b) The mean lifetimes of the metastable state $\tau_{am}$ (symbols) and inverse decay rates $R_{dqs}^{-1}$ (curves) for different values of the damping parameter $\phi$. (c) The relative difference between these two quantities according to equation (4).

4. Conclusions

For the thermal decay of a metastable state, there are two important characteristics which are often considered to be identical. First one is the mean lifetime of a Brownian particle before its escape, $\tau_{am}$; the second one is the inverse quasistationary decay rate, $R_{dqs}^{-1}$. In order to compare them, we have modeled the decay process using the Langevin dynamics. It turns out that $\tau_{am}$ is always larger than $R_{dqs}^{-1}$ for all cases under consideration. It has appeared that the presumption that $\tau_{am}$ and $R_{dqs}^{-1}$ are identical, is fulfilled within 5% only for the governing parameters $G > 4$.

For the smaller values of this parameter, the difference between $\tau_{am}$ and $R_{dqs}^{-1}$ achieves several tens percent. For example, for $G = 0.7$, it might exceed 40%. It is found that this difference significantly depends upon the damping parameter: it is 2-3 times larger for the case of the energy diffusion regime (weak damping) in comparison with the overdamping regime (strong damping). Thus, one should identify both these quantities, $\tau_{am}$ and $R_{dqs}^{-1}$, with care since they do not coincide in general.
Especially it is important in the energy diffusion regime for the comparatively small values of the governing parameters.

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