Dimensionless Universal Parameters of the Kramers Problem

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Abstract. Thermal decay of a metastable state is a useful model employed in many branches of natural sciences. The inertia parameter and friction coefficient, as well as the potential energy, might have quite a different scale in the different branches. However, the time evolution of quantities characterizing the decay process (or the Kramers problem) should be the same, e.g. the fission rate. Therefore, it is convenient to have a set of universal parameters for scaling the problem. Performing numerical modeling within the Langevin dynamics, we have managed to find such universal dimensionless parameters.

1. Introduction

Escape of a Brownian particle from a metastable state (potential well) due to thermal fluctuations appears to be a very useful model in different branches of natural sciences: chemical reactions [1,2], Josephson junction circuits [3,4], biological processes [5], and fission of excited nuclei [6–10] are several examples. Analytical formulas (approximate, of course) for the rate of thermal decay accounting for the dissipation had been published by Kramers [1]. One of these formulas obtained for weak friction (the energy-diffusion regime) was modified later in [3]. The rates calculated using the analytical formulas are compared to the numerical rates (which are supposed to be exact within the framework of statistical errors) in several articles (see, e.g. [10–12]). At some values of physical parameters, significant deviations of the approximate rates from the numerical ones are found. On the other hand, the numerical modeling often requires significant computer resources. Therefore, it seems to be useful finding scaling parameters which would allow using a decay rate obtained with one set of physical parameters for getting the rate with another set without doing new modeling. In this contribution, we report on our search for such dimensionless scaling parameters.

2. The model

We model the one-dimensional random walk of a Brownian particle using the Langevin equations (stochastic differential equations). The state of the particle is characterized by the dimensionless coordinate $q$ and the conjugate momentum $p$. The Langevin equations read [13]:

$$\frac{dp}{dt} = -\frac{\eta}{m} p + K + g\Gamma,$$

$$\frac{dq}{dt} = \frac{p}{m}. \quad (1)$$

Here $m$ and $\eta$ stand for the inertia parameter and friction coefficient, respectively. The driving force is determined by the potential energy:
The amplitude of the random force depends upon thermal energy $\theta$ (which usually is proportional to the temperature $T$):

$$g = \sqrt{\eta \theta}.$$  \hfill (4)

The random values $\Gamma$ represent white noise:

$$\langle \Gamma(t) \rangle = 0,$$

$$\langle \Gamma(t_1) \Gamma(t_2) \rangle = 2\delta(t_1 - t_2).$$  \hfill (6)

The Langevin equations (1), (2) are equivalent to the following Fokker-Planck equation for the probability density $P(q, p, t)$:

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial q} \left( \frac{p}{m} \frac{\partial P}{\partial p} \right) + \frac{\partial}{\partial p} \left[ \left( \frac{\eta}{m} p + \frac{dU}{dq} \right) \frac{\partial P}{\partial p} - \eta \theta \frac{\partial P}{\partial p} \right].$$  \hfill (7)

Since we consider the problem with the momentum independent diffusion coefficient, the Ito and Stratonovich interpretations of the Langevin equations (1), (2) coincide [14].

The potential $U(q)$ is represented by two parabolas of the same stiffness $C$ smoothly jointed at $q_m$:

$$U(q) = \begin{cases} C(q - q_c)^2/2 & \text{at } q < q_m; \\
U_b - C(q - q_b)^2/2 & \text{at } q > q_m. \end{cases}$$  \hfill (8)

The subscript “c” refers to the bottom of the potential well and “b” indicates the top of the barrier ($U_b$ denotes the barrier height). Three examples of the potential profile are shown in figure 1 (the details will be explained below).

All the trajectories begin at $q_c$ with zero momentum. The computer modeling results in $N_{tot}$ trajectories terminated not later than at the time moment $t_D$. Some of these trajectories arrive at the absorptive point $q_a$ before $t_D$. The time-dependent decay rate $R_{at}(t)$ is then evaluated as follows:

$$R_{at}(t) = \frac{1}{N_{tot} - N_{at}(t)} \frac{\Delta N_{at}}{\Delta t}.$$  \hfill (9)

Here $N_{at}(t)$ is the number of Langevin trajectories reaching $q_a$ by the time moment $t$; $\Delta N_{at}$ is the number of trajectories arriving at the absorptive point within the time interval $\Delta t$. Several examples of

Figure 1. The potentials used in the present modelling

$U_0(q)$: $\omega = \omega_0$, $U_b = U_{b0}$

$U_1(q)$: $\omega = 2 \omega_0$, $U_b = 1.33 U_{b0}$

$U_2(q)$: $\omega = 2 \omega_0$, $U_b = U_{b0}$
$R_{at}(t)$-dependences can be observed in figure 2. Omitting for the details of this picture, one sees in general that after particular transient stage the time-dependent rate stabilizes reaching a quasistationary value $R_{\text{dqs}}$. In order to calculate this rate, we use several bins backwards from the time moment $t_D$ and average the corresponding values of $R_{at}(t)$. Details of this procedure are described in [11,15].

**Figure 2.** The time-dependent decay rates for different values of the damping parameter $\varphi$ indicated in each panel and for the same value of the governing parameter $G = 2.4$. For details see discussion in section 4.
In the present contribution, we consider three potentials which are shown in figure 1. All of them are described by the same equation (8) however the constants entering this equation are different. The basic potential $U_0(q)$ possesses the barrier height $U_b = U_{b0}$ and curvature $\omega = \omega_0$; it is shown by thick curve in figure 1. The characteristics of the wider potential energy profile $U_1(q)$ displayed by the curve with triangles are $\omega = \omega_0$, $U_b = 1.33U_{b0}$. The last potential $U_2(q)$ shown by the curve with circles correspond to $\omega = 2\omega_0$, $U_b = U_{b0}$.

### 3. Scaling dimensionless parameters

Our suggestion is that changing the barrier parameters $U_b$ and/or $C$ of equation (8) and simultaneously the thermal energy $\theta$ and/or friction coefficient $\eta$, respectively, we can arrive at the same or at least close value of $R_{dqs}/\omega$.

Thus, as the first dimensionless scaling parameter of the Kramers problem we suggest the following one:

$$G = \frac{U_b}{\theta}. \tag{10}$$

We will refer to $G$ as to the governing parameter. On one hand, this is to be expected considering the approximate Kramers decay rates [1,3] since all of them are proportional to the transition state rate which reads

$$R_{TS} = \frac{\omega}{2\pi} \exp \left(-\frac{U_b}{\theta} \right). \tag{11}$$

However, these analytical formulas are valid only at extremely weak and comparatively strong dissipation. We intend to prove that $G$ is the scaling parameter for the intermediate dissipation strength as well.

The second our hypothesis is that

$$\varphi = \frac{\eta}{m\omega} \tag{12}$$

is a scaling parameter too. We will refer to it as to the damping parameter.

We would like to note that the value of the decay rate also should be scaled in order to perform the comparison. Therefore, instead of the absolute values of $R(t)$ and $R_{dqs}$, in the figures we present dimensionless values $R(t)/\omega$ and $R_{dqs}/\omega$, respectively. For the time axis we again use dimensionless quantity $t\omega$.

### 4. Results

In order to confirm our assumptions about the governing and damping parameters, we performed the modeling of the thermal decay of a metastable state for three cases with the following sets. The basic calculations were made with $U_b = U_{b0}$, $\theta = \theta_0$, $\omega = \omega_0$, and $\eta = \eta_0$. The corresponding rates are marked with subscript “0”. The decay rates with subscript “1” correspond to the case $U_b = 1.33U_{b0}$, $\theta = 1.33\theta_0$, $\omega = \omega_0$, and $\eta = \eta_0$. The decay rates with subscript “2” were obtained at $U_b = U_{b0}$, $\theta = \theta_0$, $\omega = 2\omega_0$ and $\eta = 2\eta_0$. Thus, in all these cases we keep fixed $G$ and $\varphi$ which are the candidates for the universal parameter of the Kramers problem.

Sixteen time-dependent rates $R_{at}(t)$ are shown in figure 2. The rates displayed by the lines with and without symbols are evaluated using potential energies $U_1(q)$ and $U_2(q)$, respectively. Moreover, the friction coefficient $\eta$ in the case of $U_2$ is made twice as large as the one for the case $U_1$ in order to keep the damping parameter fixed. In order to keep the governing parameter fixed as well, the thermal energy in the case of $U_1$ is taken 1.33 times larger with respect to the case of $U_2$. These pictures indicate that on the qualitative level the time-dependent decay rates are very close for different values of $U_b$, $C$ (or $\omega$), $\eta$, and $\theta$ provided the values of $G$ and $\varphi$ are fixed. Note that the quasistationary rates differ significantly: the largest value (panel (b)) more than 20 times as great as the smallest value (panel (h)). A remarkable thing is seen from the figure that not only the quasistationary values of the
rates are in accordance but the transition stages are also in a very good agreement. The typical statistical error of our calculations is 2-3%.

To perform the quantitative comparison between the rates computed with different sets of parameters, we plot the corresponding ratios in figure 3. Namely, in the upper panel there is the dimensionless decay rate calculated with the set “1” divided by the rate obtained in the basic calculations. In the lower panel the same quantity is presented but for the set “2”. This comparison is performed for the wide range of φ covering extremely weak, intermediate, and comparatively strong dissipation.

All the points in figure 3 are located close to unity. They do not demonstrate any regular dependence upon φ. Moreover, the statistical error bars for every point enter the 2% stripe near unity. Such a good agreement between the decay rates calculated for quite different conditions confirms that the chosen governing and damping parameters indeed might be considered as the universal ones.

![Figure 3](image_url)

**Figure 3.** The ratio of the dimensionless decay rates calculated with different sets of parameters as the function of damping parameter (see text for details).

5. Conclusions
The motion of Brownian particle escaping the metastable state is an effective and therefore widely used tool for describing different phenomena. Its application might be found in physics, chemistry, and biology. Therefore, the characteristics of the potential energy profile, thermal energy, friction coefficient, and inertia parameters might have significantly different scales. However, since the phenomena are based on the same model, the behaviour of the resulting quantities should be similar. Revealing of the universal parameters of the Kramers problem will allow using these similarities.

As the candidates for the universal parameters, the dimensionless governing $G$ and damping $\varphi$ parameters were chosen. The former is equal to the barrier height over the thermal energy. The latter combines the friction coefficient, inertia parameter, and curvature of the potential barrier.
For modeling the thermal decay, the one-dimensional Langevin dynamics was used. We compared the decay rates obtained with different sets of the parameter of the modeling. The time evolution of the rates, as well as their quasistationary values, were examined. For any moment of time, good agreement between the different rates was observed provided parameters $G$ and $\varphi$ were fixed; the quasistationary values differ at most by 2%. Thus, the results of our analysis confirm that the governing and damping parameters are indeed the universal ones.

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