The Kramers problem in the energy diffusion regime: transient times

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Abstract. Brownian motion driven by thermal fluctuations play an important role in the work of nanomachines and in single-molecule pulling experiments. Some problems in this field are reduced to the so-called Kramers problem concerning the decay rate of a quasistationary state. Provided all Brownian particles start their motion from the potential minimum, the rate increases in time reaching a quasistationary value. We model the process of decay using the Langevin equations. This modeling makes it possible identifying the transient time required for the rate to reach its quasistationary value. We compare the numerical transient times with those known from the literature. It turns out that the difference reaches up to 70% in the case of weak friction. Increasing friction results in decreasing this difference. In order to make our results useful for a larger audience, we present them in the dimensionless form.

1. Introduction
There are many modern examples of the Kramers problem [1] in technology and natural sciences [2-4]. Let us mention electric current through Josephson junction [5], single molecular pulling experiments [6, 7], and atomic nuclear fission [8-10]. Many studies are devoted to the quasistationary stage of the process (see e.g. [9-11]). Yet the transient stage has been investigated significantly poorer [12, 13]. In the present study we aim to obtain the dependence of the transient time upon the friction strength solving numerically stochastic differential equations (SDEs) for the energy diffusion regime.

2. Model
Following [1, 14, 15] we perform modeling for the one dimensional case. The motion of a Brownian particle is described by the dimensionless coordinate $q$ and conjugate momentum $p$. In discrete form the SDEs read:

\begin{align}
    p^{(n+1)} &= p^{(n)}(1 - \eta m^{-1} \tau) + K \tau + gb^{(n)} \sqrt{\tau}, \\
    q^{(n+1)} &= q^{(n)} + \left(p^{(n)} + p^{(n+1)}\right) \tau/(2m).
\end{align}

Here the superscripts $(n)$ and $(n + 1)$ correspond to two successive time moments separated by the time step of modeling $\tau$. The random numbers $b$ entering the random force possess a normal distribution with zero average and variance 2. In equation (1) $\eta$ and $m$ are the friction and inertia parameters, respectively; $K = -dU/dq$ represents the conservative force; $g = (\theta \eta)^{1/2}$ is the amplitude of the random force; $\theta$ is the mean thermal energy. The potential energy $U(q)$ is parametrized by two parabolas of the same stiffnesses $C$. The parabolas are smoothly joined at $q_m = 1.3$. All trajectories start from the bottom of the well at $q_c = 1.0$ with zero momentum.

The modeling results in a sequence of $N_{tot}$ trajectories terminated not later than particular time moment $t_D$. Some of the trajectories reach the absorptive border ($q_f = 2.0$) at $t < t_D$. The algorithms for finding the time dependent decay rate $R_f(t)$ and its quasistationary value $R_D$ are described in detail in [9].
3. Results
In figure 1 we present the dimensionless decay rates ($R/R_D$) versus the dimensionless time ($t\omega$) for several values of the dimensionless parameter, reflecting the value of friction

$$\varphi = \frac{\eta}{\sqrt{mC}}. \quad (3)$$

Here $\omega = (C/m)^{1/2}$. These calculations have been performed for $U_b\theta^{-1} = 3.00$ ($U_b$ is the barrier height). One clearly sees that the dynamical rates $R_{ft}(t)$ resulting from the SDEs (broken lines with symbols) are subjects of fluctuations. The quasistationary rates $R_D$ are displayed by the horizontal lines. The statistical errors of $R_D$ are about 1-2%. Finally, the smooth lines without symbols $R_m(t)$ denote the approximation of $R_{ft}(t)$; these approximations are found as explained below.

![Figure 1](image_url)

Figure 1. Time dependence of the decay rates for four values of parameter $\varphi$ indicated in the panels.

In Ref. [12] an approximate analytical expression for the dynamical rate was obtained. Its time dependence basically reads

$$R_W(t) = R_0 \exp \left\{ - \frac{U_b}{\theta h_W(t)} \right\}, \quad (4)$$

where

$$h_W(t) = 1 - \exp \left( - \frac{\eta t}{m} \right). \quad (5)$$

One sees that $R_W(t)$ approaches $R_0 \exp \{-U_b/\theta \}$ as time increases. It is natural to identify $R_0$ with $R_D \exp \{U_b/\theta \}$. However, in order to describe the transient behavior of the rate we are forced to modify equation (4) introducing an extra fitting parameter $s$:

$$R_s(t) = R_D \exp \left\{ \frac{U_b}{\theta} - \frac{U_b}{\theta h_s(t)} \right\}, \quad (6)$$

where

$$h_s(t) = 1 - \exp \left( - \frac{s \eta t}{m} \right). \quad (7)$$

The value of $s$ is chosen minimizing the deviation of $R_s(t)$ from $R_{ft}(t)$, i.e. minimizing the following value
\[ d_s = \frac{1}{n} \sum |R_s(t_i) - R_{ft}(t_i)| \]

Here \( n \) is the number of terms in the sum. In order to avoid the division by zero, the summing is performed starting from such time moment \( t_t \) that \( R_{ft}(t_t) > 0.02R_D \) for the first time. Typical dependences \( d_s(s) \) are presented in figure 2. We see that each dependence indeed possesses a well-pronounced minimum. The approximating curves \( R_m(t) \) in figure 1 are obtained with the value of \( s \) corresponding to this minimum.

In figure 3 we present the dependences of the optimum values \( s_m \) and \( d_m \) upon \( \varphi \). It turns out that \( s_m \) decreases monotonically with \( \varphi \) and reaches unity as \( \varphi \approx 0.1 \), i.e. at this value of \( \varphi \), equations (5) and (7) coincide and our results agree with Ref. [12].

Finally, we show in figure 4a the transient time \( \tau_m \) (the curve with circles) corresponding to the time moment when \( R_{ft}(t = \tau_m) = 0.90 \cdot R_D \). For comparison, we also present here the transient time \( \tau_W \) (the curve with triangles down) corresponding to equations (4), (5), i.e. to Ref. [12]. As expected, in the energy diffusion regime, the transient time decreases as friction increases, i.e. the decay process accelerates. Note, that in the opposite limiting case corresponding to the overdamping regime, the increase of friction significantly slows down the decay of a metastable state.

In figure 4b the ratio \( \tau_W/\tau_m \) is presented as a function of \( \varphi \) (the latter is proportional to the friction strength). One sees that the ratio, in fact, repeats the \( s_m(\varphi) \) – dependence presented in figure 3a. At small values of \( \varphi \), the transient time \( \tau_W \) exceeds \( \tau_m \) by almost 70%. As the value of friction increases the difference becomes significantly smaller.

4. Conclusions
In the present work we have performed numerical modeling of the thermal decay of a metastable state at small values of the friction parameter (the so-called energy diffusion regime). For this aim, the stochastic differential equations (the Langevin equations) have been used. The time dependent rates resulting from the modeling enable us extracting the transient times \( \tau_m \). It is shown that at extremely
weak friction these transient times are by 50% smaller than those known from the literature ($\tau_W$, see Ref. [12]). As the friction constant increases, our transient times approach those of [12].

Figure 4. a) Dependence of the relaxation times calculated using the analytical formulas from [12] ($\tau_W$, triangles) and extracted from the numerical simulation ($\tau_m$, circles) upon the parameter $\varphi$.

b) The ratio of these times as a function of $\varphi$.

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