Numerical modeling of the Brownian motion in a bistable potential at medium friction

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Abstract. We present results of the numerical modeling of the relaxation process for the Brownian motion in a bistable potential. Such a process is relevant for the recent nanoscale experiments reported in the literature. The modeling is based on the Langevin equations for the generalized coordinate and its conjugated momentum. First, the calculations are validated for the case of low thermal energy using a comparison with the analytical expressions for the harmonic oscillator. Next, the time evolution of the particle distribution in the bistable potential is analyzed.

1. Introduction

Nowadays, stochastic Langevin equations are widely used for modeling different natural processes from the nanometer [1] to femtometer [2,3] scales. These equations are also applied for modeling electrical systems [4]. In our previous works [5–7], we concentrated on employing these equations for describing the thermally activated decay process of a metastable state (the so-called Kramers problem, see [8–10]).

In many applications, the Brownian motion in a bistable potential is of interest. For example, in Ref. [11] the phenomenon of optical bistability (hysteresis) was discovered in the Fabry-Perot interferometer and in Ref. [12] the quantum Langevin equations were constructed for studying the behavior of the optically bistable devices. In [13], the bistable potential was realized as an optical tweezer trapping a nanoparticle. In [14], classical (not quantum) Langevin equations were used for describing the behavior of the DNA in a solvent. In [15], the dynamics of the human heart rate fluctuations was described successfully using the Langevin equations.

The Langevin equations, we are going to employ in the present work, read

\[
\frac{dp}{dt} = -\frac{dU(q)}{dq} - \frac{\eta}{m}p + g_p \Gamma, \quad #(1)
\]

\[
\frac{dq}{dt} = \frac{p}{m}. \quad #(#(2))
\]

Here \( p \) and \( q \) are the momentum and coordinate of the Brownian particle; \( U(q) \) stands for the potential energy; \( \eta \) and \( m \) are the friction and inertia parameters, respectively; \( g_p = \sqrt{\eta \theta} \) is the amplitude of the
random force in the momentum space (the thermal energy $\theta$ is related to the temperature $T$: $\theta = k_B T$; $k_B$ is the Boltzmann constant); $(\Gamma(t)) = 0$, $(\Gamma(t_1) \Gamma(t_2)) = 2\delta(t_1 - t_2)$. $\delta$ is the Dirac delta-function.

When applying the Langevin equations to the harmonic oscillator (HO), one usually deals with three regimes depending upon the value of the damping parameter $\varphi = \frac{\eta}{\omega_c m}$.$^{(3)}$

Here $\omega_c$ denotes the frequency of the oscillations near the potential minimum located at $q = q_c$. At $\varphi \ll 1$ (weak friction), the energy dissipation in one period is small and the motion is often considered as diffusion in the energy (or action) coordinate $^{[8,16]}$. The Langevin equation describing this regime was recently constructed and solved numerically $^{[17,18]}$.

At extremely strong dissipation, $\varphi \gg 1$, the motion is called overdamped $^{[8]}$. In this regime, the relaxation time of the momentum is much shorter than that of the coordinate, and two Langevin equations (1),(2) are reduced to the only equation for the coordinate

$$\frac{d q}{d t} = \frac{1}{\eta} \left[ -\frac{d U(q)}{d q} + g_p \Gamma \right].^{(4)}$$

Equation of this type is used in $^{[15,19,20]}$.

Finally, at the medium values of $\varphi$ (i.e. $\varphi \approx 1$) one deals with what we call the phase space diffusion when the relaxation time of the coordinate and momentum are of the same order. In this regime, the Langevin equations (1),(2) must be applied as it is done in $^{[7,14,21]}$.

It is interesting to see whether this hierarchy of regimes, established for the harmonic oscillator, survives for the Brownian motion in a bistable potential. This is the purpose of the present work to make some progress in this direction. More specifically, we focus on the case of medium friction leaving two other regimes for future study.

2. Model

We use the following bistable potential (see figure 1)

$$U(q) = -4U_c \left( -\frac{q^2}{2} + \frac{q^4}{4} \right) .^{(5)}$$

here $U_c = U(q_c) = -1.50$, $q_c = 1.00$, and the maximum separating two minima is located at $q = 0$.

![Figure 1. The bistable potential used in the present work.](image-url)
In the present work, for the numerical modeling we use the Euler-Maruyama algorithm [22] which reads
\begin{equation}
\begin{aligned}
\Delta p &= \left\{ -\frac{dU(q)}{dq} - \frac{\eta}{m} p \right\} h_t + g_p b \sqrt{h_t}, \#(6) \\
\Delta q &= \left( p^{(n)} + p^{(n+1)} \right) h_t / (2m). \#(9)
\end{aligned}
\end{equation}

The superscripts correspond to two moments of time separated by the time step of numerical modeling \( h_t \). In the RHS of equation (6), all quantities are taken at the time moment \( nh_t \). The random number \( b \) entering the random force possesses a normal distribution with zero average and variance equal to 2.

We consider the case when the diffusion coefficient in the momentum space, \( D_p = \eta \theta \), is momentum independent. That is why the Ito and Stratonovich interpretations of the Langevin equations (1),(2) coincide [9].

The values of constant parameters used through the present work are collected in Table 1. \( K_c \) and \( K_b \) denote the absolute values of the stiffnesses for the minima and the barrier, respectively. Parameter \( \theta \) is varied in different calculations.

**Table 1. The values of the constant parameters used in the present work**

| \( q_{ini} \) | \( p_{ini} \) | \( K_c \) | \( K_b \) | \( q_c \) | \( \varphi \) | \( \omega_b = \frac{K_b}{m} \) | \( \omega_c = \frac{K_c}{m} \) | \( U_c \) | \( m \) |
|---|---|---|---|---|---|---|---|---|---|
| 1.00 | 2.00 | 12.0 | 6.00 | 1.00 | 1.00 | 0.222 | 0.314 | -1.50 | 122 |

For all the parameters as well as for the time, the relative units are used, except the damping parameter \( \varphi \) and the coordinate \( q \) which are dimensionless. For instance, in the case of the nuclear fission process, which is relevant to the considered model, the barrier height and \( \theta \) are measured in MeV, \( [m] = \text{MeV} \cdot \text{zs}^2 \) (1 zs = 10^{-21} s), \([\eta] = \text{MeV} \cdot \text{zs} \), and \([p] = \text{MeV} \cdot \text{zs} \).

3. Testing the code: the case of harmonic oscillator

As the first step, we would like to make sure that our computer code functions correctly. This is done for \( \varphi = 0.1 \) and 1.0. \( \theta = 0.01 \). At this small value of the thermal energy (\( \theta \ll -U_c \)), the potential pocket is well approximated by the harmonic oscillator potential with the stiffness \( K_c \). The formulas for the statistics of the probability density for the HO are well known (see e.g. Appendix 1 in [23]).

The time dependence of the coordinate average \( q_{ma}(t) \) and variance \( \sigma_{qa}^2(t) \) as well as for the momentum average \( p_{ma}(t) \) and variance \( \sigma_{pa}^2(t) \) can be written as follows (the subscript ‘m’ stands for “mean” whereas ‘a’ denotes “analytical”)

\begin{equation}
\sigma_{qa}^2(t) = \sigma_{qa}^2 \left\{ e^{-\varphi \tau} \left[ \frac{\varphi^2}{4k_{\varphi}^2} \cos(2k_{\varphi} \tau) - \frac{\varphi}{2k_{\varphi}} \sin(2k_{\varphi} \tau) - \frac{1}{k_{\varphi}^2} \right] + 1 \right\}, \#(10)
\end{equation}

\begin{equation}
\sigma_{pa}^2(t) = \sigma_{pe}^2 \left\{ e^{-\varphi \tau} \left[ \frac{\varphi^2}{4k_{\varphi}^2} \cos(2k_{\varphi} \tau) + \frac{\varphi}{2k_{\varphi}} \sin(2k_{\varphi} \tau) - \frac{1}{k_{\varphi}^2} \right] + 1 \right\}, \#(11)
\end{equation}

\begin{equation}
q_{ma}(t) = q_c + \left( (q_{ini} - q_c) \varphi \frac{1}{2k_{\varphi}} \sin(k_{\varphi} \tau) + \cos(2k_{\varphi} \tau) \right) + \frac{p_{ini}}{2mk_{\varphi}^2} \sin(k_{\varphi} \tau) e^{-\varphi \tau / 2}, \#(12)
\end{equation}

\begin{equation}
p_{ma}(t) = \left\{ p_{ini} - \frac{\varphi}{2k_{\varphi}} \sin(k_{\varphi} \tau) + \cos(2k_{\varphi} \tau) \right\} - \frac{(q_{ini} - q_c) m \omega_c}{k_{\varphi}} \sin(k_{\varphi} \tau) e^{-\varphi \tau / 2}. \#(13)
\end{equation}
for $\varphi < 2$, i.e. for the phase space diffusion. Here

$$\omega_\varphi^2 = \omega_c^2 (1 - \varphi^2 / 4), \quad \tau = \omega_c t, \quad k_\varphi^2 = (1 - \varphi^2 / 4)$$

and the equilibrium values of the variances, $\sigma_{qe}^2$ and $\sigma_{pe}^2$ read

$$\sigma_{qe}^2 = \theta / (m \omega_c^2), \quad \sigma_{pe}^2 = m \theta.$$

Note, that equations (10)(11) and (11) correspond to the initial conditions $\sigma_q^2(0) = 0, \sigma_p^2(0) = 0$. Another thing that must be noticed is that the equilibrium value of $\sigma_p^2$ does not depend upon $\omega_c$ and, in fact, upon the shape of the potential.

The results of the modeling are compared with the analytical formulas (10)(11), (11) in figure 2 at $\varphi = 1.0$. Note, that in this example about $10^{11}$ random numbers were generated. For this aim, a generator based on “long integer” values of C-language was used [24]. Mean (‘m’) numerical (‘n’) values and variances are in good agreement with the analytical ones confirming the accuracy of our code.

**Figure 2.** As functions of time, the following quantities obtained numerically are displayed by symbols: a) numerical momentum variance $\sigma_{p,n}^2(t)$; b) numerical mean momentum $p_{mn}(t)$; c) numerical coordinate variance $\sigma_{q,n}^2(t)$; d) numerical mean coordinate $q_{mn}(t)$. Thin lines correspond to the analytical values, thick horizontal lines are for the equilibrium values for the HO at $q = q_c$. In panel c) all quantities are multiplied by $10^3$. $\theta = 0.01$. 
4. Results

Now we model the Brownian motion in the bistable potential shown in figure 1 using equations (6)-(9) with the following initial conditions for the coordinate and momentum, respectively: $q_{ini} = q_e$, $p_{ini} = 2.00$. The latter value is to be compared with

$$p_b = \sqrt{-2mU_c} = 19.1$$

which corresponds to the minimum momentum required to overcome the barrier in the absence of dissipation. The values of other variable parameters are $\theta = 0.50$, $\varphi = 1.00$.

4.1. Relaxation of the momentum and the coordinate in the right pocket

For the case of medium dissipation considered in the present work, one expects two relaxation processes in this potential. First, relaxation of the momentum and the coordinate in the right pocket should happen during the commensurable time lapses. The characteristic time of this processes is the relaxation time of the momentum variance

$$t_p = \frac{m}{\eta}$$

Results of the numerical modeling presented in figure 3 confirm this expectation. In figure 3a) the momentum variance reaches its equilibrium value after several $t_p = 3.18$. Deviations of $\sigma^2_{p_{na}}(t)$ from $\sigma^2_{p_{na}}(t)$ (the latter is for the harmonic oscillator) are because at comparatively high temperature ($\theta = -0.33U_c$) the Brownian particles feel the anharmonicity of the potential.

In figure 3b) one sees that the mean numerical momentum $p_{mn}(t)$ takes twice as long for its relaxation. Moreover, at $t \gg 2t_p$ the average momentum does not approach zero as one expects for
the HO (see equation (13)). The small negative quasistationary value of $p_{mn}$ observed in figure 3b) corresponds to the quasistationary probability flux to the left well. Due to this flux, the coordinate variance in figure 3c) increases whereas the coordinate average in figure 3d) decreases not showing any saturation.

4.2. Equilibration of the coordinate probability density in both wells

The second relaxation process is establishing an equilibrium coordinate distribution filling both wells. For the bistable potential analytical formulas similar to equations (10)(11), (11) absent in the literature. One only has the stationary (equilibrium) probability density which reads

$$\rho_{eq}(q) = C_n \exp\left\{ \frac{U(q)}{\theta} \right\}. \#(18)$$

Here $C_n$ is the normalization constant. In figure 4, we see that the number of particles in the right well decreases and consequently this number increases in the left well. Thus, the calculated probability density approaches the equilibrium one becoming rather close to the latter at a large value of time ($t = 1600$). Obviously, at the equilibrium the probabilities to find a Brownian particle in the right or in the left well are equal to 50%.

![Figure 4. The time-dependent numerical probability densities (symbols) for several time moments (indicated in the figure) are compared with the equilibrium probability density (line without symbols). $\theta = 0.5$.](image)

To estimate the time of this relaxation process, it is convenient applying the Kramers formula [8] which can be written as follows

$$t_K = \left\{ \frac{\omega_c^2}{2\pi \omega_b} \exp\left( \frac{U_c}{\theta} \right) \left[ \left( \frac{\varphi^2}{4} + \frac{\omega_b^2}{\omega_c^2} \right)^{1/2} - \frac{\varphi}{2} \right] \right\}^{-1} . \#(19)$$

In fact, this formula was derived in [8] for the quasistationary rate and should be applied for the average decay time with care (see e. g. [5,25]). Moreover, this formula is correct only when the well, where the flux runs to, is nearly empty. Otherwise, the backward flux appears, and the net equilibration process slows down. One faces a similar problem in the nuclear fission process in the presence of the double-
humped barrier [26,27]. For our example, \( t_K = 776 \). This value does not contradict the time evolution of the numerical probability densities presented in figure 4.

Knowing the relaxation time, it is possible evaluating analytically the probability to find the Brownian particle in the right well provided it was there in the initial moment of time:

\[
\Pi_a(t) = \frac{N_r(0)}{N_{tot}} \exp\left(-\frac{t}{t_K}\right). \tag{20}
\]

Here \( N_r(0) \) is number of particles located at the right well at the initial moment of time whereas \( N_{tot} \) is the total number of Brownian particles. One should keep in mind that in equation (19) it is supposed that the decay process starts at \( t = 0 \). In our calculations, the process starts after the relaxation of the coordinate and momentum in the right well whose characteristic time is \( t_p \) (see equation (17)). Therefore, the corrected probability accounting for this delay reads

\[
\Pi_{ac}(t) = \frac{N_r(0)}{N_{tot}} \exp\left(-\frac{t - 3t_p}{t_K}\right). \tag{21}
\]

It is compared in figure 5 with the numerical probability \( \Pi_n(t) \) which is defined as

\[
N_r(t) = N_{tot} \int_0^\infty \rho(q) dq. \tag{22}
\]

One sees that the analytical (curve) and numerical (symbols) values at \( t < 150 \) agree with each other very well. At large moments of time, the symbols start deviating significantly due to the fact that the left well is not empty anymore. The number of particles in the left well increases with time; as a result, the deviation becomes larger and \( \Pi_n \) reaches 50% at \( t > 2t_K \) (see figure 4 for comparison).

\[\text{Figure 5. The analytical (curve, equation (21)) and numerical (symbols) probability of finding Brownian particle in the right well as functions of time.}\]
5. Conclusions
In the present work, the numerical modeling of the thermally activated decay of a metastable state in a bistable potential is performed. This potential is of interest for many technical and biological applications like optical tweezer and Fabry-Perot interferometer or investigations with DNA in a solvent.

The Langevin equations for the generalized coordinate and conjugated momentum are applied for this modeling. First, we test our model by analyzing the time evolution of the particle distribution obtained numerically at low thermal energy. In this case, the calculations using bistable potential with the initial condition $\rho(q) = N_{tot}\delta(q - q_c)$ are equivalent to the calculations in the harmonic oscillator potential for which the analytical formulas exist. Comparison of the numerical and analytical results shows good agreement.

Next, we present the time evolution of the particle distribution within the bistable potential at higher thermal energy. We analyze the time behavior of the probability density statistics (average values and variances). Finally, we evaluate the probability of finding a Brownian particle in the right well (where it is located at the initial moment of time). While the left well is almost empty, the numerical probability agrees with the one extracted from the classical Kramers result (see Eq. (19)).

Thus, we have analyzed numerically the behavior of the Brownian particles in the bistable potential and have demonstrated its consistency. In the future, we plan to expand our investigation to make it possible to compare the numerical results with the values observed in the experiments.

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