Stochastic thermodynamics for a diffusion process in a parabolic potential

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Abstract

In this study, we investigate the motion of a Brownian particle in a parabolic potential that varies in time. We consider the one-dimensional motion of this particle and solve the Langevin equation for two random variables - position and velocity. As there is no analytical solution for a general time-dependent potential, we introduce a formal solution using time-ordered exponential. We then obtain the solution to the Smoluchowski equation, whose result is the probability density of the particle in the phase space. For a constant potential, we find an explicit solution and derive a recursive formula for the case of piecewise-constant potential.

1 Introduction and model setting

We consider one-dimensional Brownian motion of a single particle in an external time-dependent parabolic potential,

$$U(x,t) = \frac{1}{2}k(t)x^2. \tag{1}$$

Here $k(t)$ describes the externally controlled elastic parameter. In the following we designate $\gamma(t) = k(t)/m$, where m is the mass of the Brownian particle. Below, the function $\gamma(t)$ is referred as the driving protocol.

First, in the second Sec. we give result which are valid for an arbitrary driving protocol. Unfortunately, a fully-closed form of the solution is only accessible for particular functional forms of the driving protocol.

In the third Sec. we develop a recursive scheme which yield the full solution for a piecewise-constant driving protocol. As such, it can be used for to approximate an arbitrary time-domain external driving protocol

Due to the assumed thermal force, the velocity and the position of the particle are stochastic functions and they are described by a system of Langevin equations.

Alternatively, the dynamics is described by the simultaneous probability density for the particle position and its velocity. Assuming that the thermal force is described by the Gaussian white noise, the probability density is dictated by the Smoluchowski equation.

The central objective of the present work is the solution of the above equation

$$\ddot{\mathsf{X}}(t) = -\beta\dot{\mathsf{X}}(t) - \gamma(t)\mathsf{X}(t) + \mathsf{A}(t), \tag{2}$$

where $\mathsf{A}(t)$ is the thermal force (Gaussian white noise) divided by the mass of the Brownian particle. The correlation function $\mathsf{A}(t)$ satisfies the equality $\langle \mathsf{A}(t)\mathsf{A}(t')\rangle = 2q\delta(t-t')$ and $\langle \mathsf{A}(t)\rangle = 0$. Here and bellow this brackets $\langle . \rangle$ means probabilistic averaging. From fluctuation-disipation theorem $q = k_B T\beta/m$ (k_B is the Boltzmann constant and T is temperature) and β is the coefficient of friction.

2 Arbitrary driving protocol

In this section, we will consider the motion of a particle in a parabolic potential, where the driving protocol $\gamma(t)$ is a given function of time. Initial condition x_0 and u_0 is imposed at time t_0.

2.1 Deterministic evolution

First of all, let us consider the dynamics without the thermal force $\mathsf{A}(t)$. It is dictated by the Newton equations of motion

$$\dot{x}(t) = u(t), \tag{3}$$

$$\dot{u}(t) = -\beta u(t) - \gamma(t)x(t). \tag{4}$$

The matrix form of the equation is given by

$$\frac{d}{dt}\mu(t) = -\mathbb{H}(t)\mu(t), \tag{5}$$

where $\mathbb{H}(t)$ is the corresponding matrix of the system

$$\mathbb{H}(t) = \begin{pmatrix} 0 & -1 \\ \gamma(t) & \beta \end{pmatrix}, \qquad \mu(t) = \begin{pmatrix} x(t) \\ u(t) \end{pmatrix}.$$

Formally this system can be solved using time-ordered exponential

$$\mathbb{E}(t, t_0) := \underset{\longleftarrow}{\exp}\left\{ -\int_{t_0}^{t} dt' \mathbb{H}(t') \right\}, \tag{6}$$

where $\underset{\longleftarrow}{\exp}$ denotes the time-ordered exponential. The solution has the form

$$\mu(t, t_0, \mu_0) := \mathbb{E}(t, t_0)\mu_0, \qquad \mu_0 = \begin{pmatrix} x_0 \\ u_0 \end{pmatrix}.$$

The evolution operator $\mathbb{E}(t, t_0)$ satisfies that for any $s \in (t, t_0)$, it holds that $\mathbb{E}(t, t_0) = \mathbb{E}(t, s)\mathbb{E}(s, t_0)$. In Section three this will enable us to compose the evolution operator. The evolution operator can be compute explicitly for exapmple for constant driving protocol $\gamma(t) = \gamma$ =const.

$$\mathbb{E}(t,t_0) = \frac{1}{\lambda^+ - \lambda^-}\begin{pmatrix} \lambda^+ e^{\lambda^- s} - \lambda^- e^{\lambda^+ s} & e^{\lambda^+ s} - e^{\lambda^- s} \\ -\lambda^+\lambda^-(e^{\lambda^+ s} - e^{\lambda^- s}) & \lambda^+ e^{\lambda^+ s} - \lambda^- e^{\lambda^- s} \end{pmatrix} \tag{7}$$

where $\lambda^{\pm} = \frac{1}{2}(-\beta \pm \sqrt{\beta^2 - 4\gamma})$ eigenvalues of matrix $\mathbb{H}$ and $s = t - t_0$.

2.2 Langevin equation and its solution

Let us now include the thermal force. Then the position $\mathsf{X}(t)$ and the velocity $\mathsf{U}(t)$ of the particle becomes stochastic function and their evolution is defined by the system of the Langevin equation

$$\dot{\mathsf{X}}(t) = \mathsf{U}(t), \tag{8}$$

$$\dot{\mathsf{U}}(t) = -\beta\mathsf{U}(t) - \gamma(t)\mathsf{X}(t) + \mathsf{A}(t). \tag{9}$$

Let us denote $\mathcal{M}(t) = (\mathsf{X}(t), \mathsf{U}(t))^+$ and $\mathcal{A}(t) = (0, \mathsf{A}(t))^+$. We obtain a nonhomogeneous equation

$$\frac{d}{dt}\mathcal{M}(t) = -\mathbb{H}(t)\mathcal{M}(t) + \mathcal{A}(t), \tag{10}$$

and its solution

$$\mathcal{M}(t,t_0,\mu_0) := \mu(t,t_0,\mu_0) + \int_{t_0}^{t} dt'\mathbb{E}(t,t')\mathcal{A}(t'). \tag{11}$$

It is now seen that by averaging the solution, using $\langle \mathsf{A}(t) \rangle = 0$, we obtain $\mu(t,t_0,\mu_0) = \langle \mathcal{M}(t,t_0,\mu_0) \rangle$.

2.3 Smoluchowski equation and its solution

In this section, we focus on constructing the function $\mathcal{G}(t,\eta,t_0,\mu_0)$ where $\eta = (x,u)^+$. This function is conditional simultaneous probability density for the random variable $\mathsf{X}(t)$ and $\mathsf{U}(t)$. The function describes probability density for the particle's presence in the phase space, whose motion is described by the Langevin equations. The density is defined as

$$\mathcal{G}(t,\eta,t_0,\mu_0)dxdy = \mathrm{Prob}\big\{\mathsf{X}(t) \in (x{+}dx) \wedge \mathsf{U}(t) \in (u{+}du) | \mathcal{M}(t_0) = \mu_0\big\}. \tag{12}$$

This function solves the Smoluchowski equation

$$\frac{\partial}{\partial t}\mathcal{G}(t,\eta) + u\frac{\partial}{\partial x}\mathcal{G}(t,\eta) = \frac{\partial}{\partial u}\left((\beta u - \gamma(t)x)\mathcal{G}(t,\eta)\right) + q\frac{\partial^2}{\partial u^2}\mathcal{G}(t,\eta), \tag{13}$$

with initial condition $\mathcal{G}(t_0,\eta) = \delta(\mu_0 - \eta)$. We could try to find a solution directly. However, we develop the solution in different way.

Probability density of a particle's occurrence in the phase space, whose motion is governed by the system of Langevin equation 10, is a Gaussian distribution [17](in our case bi-variate Gaussian distribution). The Gaussian distribution is determined by the correlation matrix and the mean value vector. Now we know, that density function $\mathcal{G}(t,\eta,t_0,\mu_0)$ have the form

$$\mathcal{G}(t,\eta,t_0,\mu_0) = \frac{1}{2\pi\sqrt{\det\mathbb{V}(t,t_0)}}\exp\left\{-\frac{1}{2}(\eta-\mu(t,t_0,\mu_0))^{+}\mathbb{V}^{-1}(t,t_0)(\eta-\mu(t,t_0,\mu_0))\right\}. \tag{14}$$

Where $\mu(t,t_0,\mu_0)$ is the mean value vector and $\mathbb{V}(t,t_0)$ is the correlation matrix. It can be shown that the function $\mathcal{G}(t,\eta,t_0,\mu_0)$ is a solution of the Smoluchowski equation. All we need is to find the correlation matrix.

The correlation matrix $\mathbb{V}(t,t_0)$ is defined as

$$\mathbb{V}(t,t_0) := \big\langle \mathcal{M}(t,t_0,\mu_0)\mathcal{M}^{+}(t,t_0,\mu_0)\big\rangle - \big\langle \mathcal{M}(t,t_0,\mu_0)\big\rangle\big\langle \mathcal{M}^{+}(t,t_0,\mu_0)\big\rangle. \tag{15}$$

We substitute from the solution (10) for $\mathcal{M}(t,t_0,\mu_0)$ and get

$$\begin{aligned}\big\langle \mathcal{M}(t,t_0,\mu_0)\mathcal{M}^{+}(t,t_0,\mu_0)\big\rangle &= \mu(t,t_0,\mu_0)\mu^{+}(t,t_0,\mu_0)+ \\ &+\int_{t_0}^{t} dt'\int_{t_0}^{t} dt''\big\langle \mathsf{A}(t')\mathsf{A}(t'')\big\rangle\mathbb{E}(t,t')\mathbb{Q}\mathbb{E}^{+}(t,t'').\end{aligned}$$

Where $\mathbb{Q} = \mathrm{diag}(0,1)$ is diagonal matrix. The correlation function of white noise, as mentioned in the introduction, is a delta distribution $\big\langle \mathsf{A}(t')\mathsf{A}(t'')\big\rangle = 2\delta(t'-t'')q$, this equality allows us to calculate the integral with respect to t'' using the delta function. Since the mean value vector is equal to the deterministic evolution we have the following equality $\big\langle \mathcal{M}(t,t_0,\mu_0)\big\rangle\big\langle \mathcal{M}(t,t_0,\mu_0)^{+}\big\rangle = \mu(t,t_0,\mu_0)\mu^{+}(t,t_0,\mu_0)$, by subtracting this equality from the equation above, we obtain the correlation matrix. The result is

$$\mathbb{V}(t,t_0) = 2q\int_{t_0}^{t} dt'\mathbb{E}(t,t')\mathsf{QE}^{+}(t,t'). \tag{16}$$

We can see that $\mathbb{V}(t,t_0)$ is independent of the initial condition μ_0. The correlation matrix is symmetric and positive definite.

The property of correlation matrix is that for any $s \in (t_0,t)$, it holds that

$$\mathbb{V}(t,t_0) = \mathbb{V}(t,s) + \mathbb{E}(t,s)\mathbb{V}(s,t_0)\mathbb{E}^{+}(t,s) \tag{17}$$

This equality is called the correlation matrix decomposition theorem. This theorem will be useful in constructing a differential equation for the correlation matrix, or, in the third Sec. for finding solutions of piecewise-constant protocols.

If we consider the decomposition of the correlation matrix $\mathbb{V}(t+\epsilon,t_0)$ and set $s=t$ we obtain this equality

$$\mathbb{V}(t+\epsilon,t_0) = \mathbb{V}(t+\epsilon,t) + \mathbb{E}(t+\epsilon,t)\mathbb{V}(t,t_0)\mathbb{E}^{+}(t+\epsilon,t). \tag{18}$$

From the Taylor expansion, we have $\mathbb{E}(t+\epsilon,t) = \mathbb{I} - \epsilon\mathbb{H}(t) + \mathcal{O}(\epsilon^2)$ and $\mathbb{V}(t+\epsilon,t) = 2q\int_t^{t+\epsilon} dt'\mathbb{E}(t,t')\mathsf{QE}^+(t,t') = 2q\int_t^{t+\epsilon} dt'\mathbb{Q} + \mathcal{O}(\epsilon) = 2q\mathbb{Q}\epsilon + \mathcal{O}(\epsilon^2)$. It leads to the equation

$$\mathbb{V}(t+\epsilon,t_0) = 2q\mathbb{Q}\epsilon + \mathbb{V}(t,t_0) - \epsilon\mathbb{H}(t)\mathbb{V}(t,t_0) - \epsilon\mathbb{V}(t,t_0)\mathbb{H}^+(t) + \mathcal{O}(\epsilon^2) \tag{19}$$

and

$$\frac{d}{dt}\mathbb{V}(t,t_0) = 2q\mathbb{Q} - \mathbb{H}(t)\mathbb{V}(t,t_0) - \mathbb{V}(t,t_0)\mathbb{H}(t). \tag{20}$$

This is a nonhomogeneous system of three differential equations with non-constant coefficients for the correlation matrix.

3 Piecewise-constant driving protocol

In this section, we consider a piecewise-constant driving protocol.

Let $\gamma(t)$ be a piecewise-constant driving protocol exhibiting n jumps in the time interval (t_0,t) at time instants $t_0,...,t_n$ with $t_0 < t_1 < t_2 < ... < t_n < t$, $\gamma(t) = \gamma_j$ in each time segment (t_j,t_{j+1}). This driving protocol can be written as

$$\gamma(t) = \gamma_0 + \sum_{j=1}^{n}(\gamma_j - \gamma_{j-1})\Theta(t-t_j), \tag{21}$$

where $\Theta(t-t_j)$ is the Heaviside step function ($\Theta(x) = 1$ for $x \geq 0$ and zero otherwise). The duration of the i-th segment is denoted as $s_i = t_{i+1} - t_i$.

3.1 Evoluion operator

In the case of a constant driving protocol γ_i, the operator $\mathbb{E}_i(t_{i+1},t_i)$ (and last last of n-th segment $\mathbb{E}_n(t,t_n)$) has an explicit form. For the i-th segment, we obtain the equation:

$$\frac{d}{dt}\mathcal{M}(t) = -\mathbb{H}_i\mathcal{M}(t) + \mathcal{A}(t) \tag{22}$$

where

$$\mathbb{H}_i = \begin{pmatrix} 0 & -1 \\ \gamma_i & \beta \end{pmatrix} \tag{23}$$

Now we can explicitly compute the expression for the operator $\mathbb{E}_i(t_{i+1},t_i) = \exp(-\mathbb{H}_i s_i)$ for the i-th segment. Let's denote $\lambda_i^\pm = \frac{1}{2}(-\beta \pm \sqrt{\beta^2 - 4\gamma_i})$ eigenvalues of matrix $\mathbb{H}_i$. We define the evoluion operator $\mathbb{S}_i$ of i-th segment as

$$\mathbb{S}_i := \frac{1}{\lambda_i^+ - \lambda_i^-}\begin{pmatrix} \lambda_i^+ e^{\lambda_i^- s_i} - \lambda_i^- e^{\lambda_i^+ s_i} & e^{\lambda_i^+ s_i} - e^{\lambda_i^- s_i} \\ -\lambda_i^+\lambda_i^-(e^{\lambda_i^+ s_i} - e^{\lambda_i^- s_i}) & \lambda_i^+ e^{\lambda_i^+ s_i} - \lambda_i^- e^{\lambda_i^- s_i} \end{pmatrix}. \tag{24}$$

The matrix $\mathbb{S}_i$ is given by $\mathbb{E}(t,t_0)$ in Sec. Deterministic evolution for constant protocol with $\gamma = \gamma_i$ and $s = s_i = t_{i+1} - t_i$. The evolution operator for a constant protocol depends only on the time difference, so we can write $\mathbb{E}_i(t_{i+1},t_i) = \mathbb{E}_i(s_i) = \mathbb{S}_i$

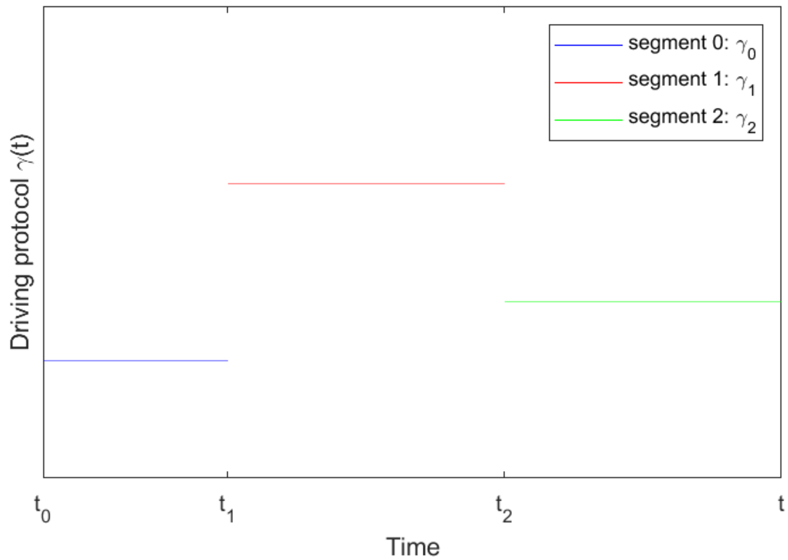

Figure 1: Figure shows values of piecewise-constant driving protocol $\gamma(t)$ exhibit two jumps in time interval $[t_0, t]$, so there is three segments.

In this section, we will denote $\mathbb{E}(t, t_0) := \mathbb{E}^{(n)}$ as the evoluion operator where there were n jumps. For example

$$\mathbb{E}(t, t_0) := \mathbb{E}^{(n)} = \mathbb{S}_n \mathbb{S}_{n-1} \dots \mathbb{S}_2 \mathbb{S}_1 \mathbb{S}_0. \tag{25}$$

Therefore, we are describing $n+1$ segments. For further purposes, let us denote

$$\mathbb{F}^{(n,i)} := \mathbb{S}_n \mathbb{S}_{n-1} \dots \mathbb{S}_{i+3} \mathbb{S}_{i+2} \mathbb{S}_{i+1}, \qquad \mathbb{F}^{(n,n)} := \mathbb{I}$$

where $\mathbb{I}$ is identity operator.

The picture 2 and 3 shows $\mathsf{X}(t)$, $\mathsf{U}(t)$ and the analytically calculated values of $\langle \mathsf{X}(t) \rangle$ and $\langle \mathsf{U}(t) \rangle$ with one jump. The initial condition was set $\mu_0 = (3, -2)^+$.

3.2 Correlation matrix

Similar to the section about the evoluion operator for the i-th segment, we can create the correlation matrix of the i-th segment and from it the complete correlation matrix for the entire interval (t_0, t). To construct the complete correlation matrix, we will utilize the theorem of decomposition. First, let us define the correlation matrix of the i-th segment $\mathbb{W}_i$ in the following way

$$\mathbb{W}_i := \mathbb{V}_i(t_{i+1}, t_i) = 2q \int_{t_i}^{t_{i+1}} dt' \mathbb{E}_i(t_{i+1}, t') \mathsf{Q} \mathsf{E}_i^+(t_{i+1}, t') \tag{26}$$

And last matrix is $\mathbb{W}_n = \mathbb{V}_n(t, t_n)$. Explicitly

$$\mathbb{W}_i := \mathbb{V}_i(t_{i+1}, t_i) = \frac{2q}{(\lambda_i^+ - \lambda_i^-)^2} \cdot$$

$$\cdot \begin{pmatrix} \frac{e^{2\lambda_i^- s_i}-1}{2\lambda_i^-} + \frac{e^{2\lambda_i^+ s_i}-1}{2\lambda_i^+} - \frac{2e^{(\lambda_i^- + \lambda_i^+)s_i}-2}{\lambda_i^- + \lambda_i^+} & \frac{1}{2}(e^{\lambda_i^+ s_i} - e^{\lambda_i^- s_i})^2 \\ \frac{1}{2}(e^{\lambda_i^+ s_i} - e^{\lambda_i^- s_i})^2 & \frac{\lambda_i^-(e^{2\lambda_i^- s_i}-1)+\lambda_i^+(e^{2\lambda_i^+ s_i}-1)}{2} - \frac{2\lambda_i^+\lambda_i^-(e^{(\lambda_i^+ + \lambda_i^-)s_i}-1)}{\lambda_i^+ + \lambda_i^-} \end{pmatrix} \tag{27}$$

From the theorem of decomposition of the correlation matrix for a single jump of the driving protocol $\gamma(t)$ (i.e., for two segments), we obtain the complete correlation matrix $\mathbb{V}(t, t_0)$

$$\mathbb{V}(t, t_0) = \mathbb{V}^{(1)} = \mathbb{W}_1 + \mathbb{S}_1 \mathbb{W}_0 \mathbb{S}_1^+ \tag{28}$$

As mentioned above for the evoluion operator, we denote the number of jumps of the driving protocol as a superscript for the correlation matrix $\mathbb{V}(t, t_0) = \mathbb{V}^{(n)}$. This yields a recursive formula for the correlation matrix.

$$\mathbb{V}^{(n+1)} = \mathbb{W}_{n+1} + \mathbb{S}_{n+1} \mathbb{V}^{(n)} \mathbb{S}_{n+1}^+ \tag{29}$$

Explicitly

$$\mathbb{V}^{(n)} = \sum_{i=0}^{n} \mathbb{F}^{(n,i)} \mathbb{W}_i (\mathbb{F}^{(n,i)})^+ \tag{30}$$

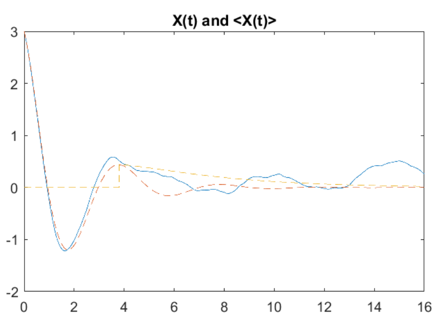

Figure 2: This figure shows $\mathsf{X}(t)$ (blue line) and its $\langle \mathsf{X}(t) \rangle$ represented by a dashed line. In segment 0, (time interval $[0, 3.8]$) the parameters are set to values of $\gamma_0 = 4$, $\beta = 1$, and $q = 0.15$. In segment 1, (time interval $(3.8, 16]$), the parameters are set to values of $\gamma_1 = 0.3$, $\beta = 1$, and $q = 0.15$.

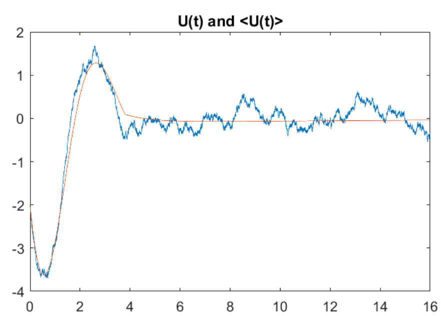

Figure 3: This figure shows the corresponding velocity $\mathsf{U}(t)$ and $\langle \mathsf{U}(t) \rangle$ of a Brownian particle, whose position is shown in Figure 2.

4 Summary and perspectives

In this study, we have investigated the motion of a Brownian particle in a parabolic potential with time-dependent driving protocol. We focused on the one-dimensional motion of the particle and solved the Langevin equation for the position and velocity variables. Due to the absence of an analytical solution for a general time-dependent driving protocol, we introduced a formal solution using the time-ordered exponential 6.

The main objective of this work was to solve the Smoluchowski equation, which describes the dynamics of the particle 13. By obtaining the solution to the Smoluchowski equation, we determined the probability density of the particle in the phase space 14. For a constant potential, we derived an explicit solution represented by 7 and 27, and for the case of a piecewise-constant protocol, we developed a recursive scheme 29 and explicit formula 30.

The obtained results for a constant or piecewise-constant protocol remain valid even in the case of complex eigenvalues $\lambda_i^{\pm}$ of the matrix $\mathbb{H}$ or negative values of γ. This allows us to examine solutions where the mean values of $\langle \mathsf{X}(t) \rangle$ and $\langle \mathsf{U}(t) \rangle$ oscillate or diverge from the center. Furthermore, it is possible compute the mean value of $\langle \mathsf{X}^2(t) \rangle$ from correlation matrix to determine the average work performed by the system.

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