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Derivation of diffusion coefficient of a Brownian particle in tilted periodic potential from the coordinate moments

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ABSTRACT

In this research, diffusion of an overdamped Brownian particle in the tilted periodic potential is investigated. Using the one-dimensional hopping model, the formulations of the mean velocity V_N and effective diffusion coefficient D_N of the Brownian particle have been obtained [B. Derrida, J. Stat. Phys. 31 (1983) 433]. Based on the relation between the effective diffusion coefficient and the moments of the mean first passage time, the formulation of effective diffusion coefficient D_{eff} of the Brownian particle also has been obtained [P. Reimann, et al., Phys. Rev. E 65 (2002) 031104]. In this research, we'll give another analytical expression of the effective diffusion coefficient D_{eff} from the moments of the particle's coordinate.

1. Introduction

Thermal diffusion in a tilted periodic potential plays a prominent role in physical [1–3] and biophysical processes [4–6]. To this diffusion, we are very interested in their mean velocity V and effective diffusion coefficient D_{eff}. In many cases, thermal diffusion can be modeled as overdamped Brownian motion

$$\xi\frac{dx(t)}{dt} = -\frac{\partial\Phi(x)}{\partial x} + \sqrt{2k_BT\xi}\, f_B(t), \tag{1}$$

where ξ is viscous friction coefficient, k_B is Boltzmann's constant, $\Phi(x)$ is a tilted periodic potential with period L, T is absolute temperature and $f_B(t)$ is Gaussian noise. Based on the relation between the effective diffusion coefficient and the first two moments of the mean first passage time (MFPT), the mean velocity and effective diffusion coefficient can be expressed in quadratures [7,8]

$$V = \frac{1-e^{\frac{\Delta\Phi}{k_BT}}}{\int_0^L dx\, I_+(x)}L, \qquad D_{\text{eff}} = \frac{\int_0^L dx\, I_+^2(x)I_-(x)}{\left[\int_0^L dx\, I_+(x)\right]^3}DL^2, \tag{2}$$

where

$$I_\pm = \mp\frac{e^{\pm\Phi(x)/K_BT}}{D}\int_x^{x\mp L} dy\, e^{\mp\Phi(y)/K_BT} \tag{3}$$

$\Delta\Phi \triangleq \Phi(L)-\Phi(0)$ and D is the free diffusion constant of Brownian particles, which satisfies the Einstein relation $D = k_BT/\xi$.

At the same time, for an one-dimensional hopping model with N states having occupation probabilities p_j and arbitrary transition rates u_j and w_j [9]

$$\frac{\partial p_j(t)}{\partial t} = u_{j-1}p_{j-1}(t) + w_{j+1}p_{j+1}(t) - [u_j + w_j]p_j(t),$$
$$0 \leqslant j \leqslant N. \tag{4}$$

Derrida [9] has obtained the exact steady-state behavior. The mean velocity of (4) is

$$V = \frac{L}{R_N}\left(1 - \prod_{j=0}^{N-1}\frac{w_j}{u_j}\right), \tag{5}$$

where

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$$R_N = \sum_{j=0}^{N-1} r_j, \quad r_j = \frac{1}{u_j}\left[1 + \sum_{k=1}^{N-1} \prod_{i=j+1}^{j+k} \frac{w_i}{u_i}\right]. \tag{6}$$

The effective diffusion coefficient of (4) is

$$D_N = \frac{L}{N}\left[\frac{LU_N + VS_N}{R_N^2} - \frac{(N+2)V}{2}\right], \tag{7}$$

where

$$S_N = \sum_{j=0}^{N-1} s_j \sum_{k=0}^{N-1} (k+1) r_{k+j+1}, \qquad U_N = \sum_{j=0}^{N-1} u_j r_j s_j, \tag{8}$$

$$s_j = \frac{1}{u_j}\left[1 + \sum_{k=1}^{N-1} \prod_{i=j-1}^{j-k} \frac{w_{i+1}}{u_i}\right]. \tag{9}$$

Although the analytic expression (2) for effective diffusion coefficient D_{eff} of Brownian particles already exists, its derivation is based on the first two moments of the first passage time [7]. Yet, the typical experimental procedure to determine the diffusion coefficient relies on the long-time behaviour of the first two moments of the particle's coordinate [10,11]. Therefore, it is interesting from the fundamental viewpoint to derive D_{eff} theoretically based on the coordinate moments rather than passage time moments. In this research, we'll derive the analytical expression of the mean velocity and effective diffusion coefficient of Brownian particles from this point of view.

It is well known that the motion of Brownian particles also can be described by the following Fokker–Planck equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\rho}{\xi}\frac{\partial \Phi}{\partial x} + D\frac{\partial \rho}{\partial x}\right), \quad -\infty < x < \infty, \tag{10}$$

where $\rho(x,t)$ is the density of the probability of Brownian particles at position x and time t. In the following, we'll give the formulations of the mean velocity and effective diffusion coefficient under the assumptions similar to those used in the derivation of Derrida to get the velocity and dispersion of the one-dimensional hopping model [9]. Our expression for the effective diffusion coefficient is approximate and therefore not equivalent to the exact result (2). But the numerical calculations indicate that the difference between the two expressions is small. In other words, our formulation is a good approximation to the real one.

2. The mean velocity and effective diffusion coefficient

2.1. The mean velocity

Similar to the discussion in [9], let

$$\bar{R}(x,t) = \sum_{k=-\infty}^{+\infty} \rho(x+kL,t),$$

$$\bar{S}(x,t) = \sum_{k=-\infty}^{+\infty} (x+kL)\rho(x+kL,t), \quad 0 \leqslant x \leqslant L. \tag{11}$$

It can be verified that

$$\bar{R}(x+L,t) = \bar{R}(x,t), \qquad \bar{S}(x+L,t) = \bar{S}(x,t),$$

$$\int_0^L \bar{R}(x+L,t)\,dx = 1,$$

$$\frac{\partial \bar{R}}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\bar{R}}{\xi}\frac{\partial \Phi}{\partial x} + D\frac{\partial \bar{R}}{\partial x}\right), \quad 0 \leqslant x \leqslant L, \tag{12}$$

and

$$\frac{\partial \bar{S}}{\partial t} = \sum_{k=-\infty}^{+\infty} (x+kL)\frac{\partial \rho(x+kL,t)}{\partial t}$$
$$= \frac{1}{\xi}\left\{\frac{\partial}{\partial x}\left(\bar{S}\frac{\partial \Phi}{\partial x} + k_B T\frac{\partial \bar{S}}{\partial x} - k_B T\bar{R}\right) - \left(\bar{R}\frac{\partial \Phi}{\partial x} + k_B T\frac{\partial \bar{R}}{\partial x}\right)\right\}. \tag{13}$$

Similar to [9], we assume that in the steady state

$$\lim_{t\to\infty} \bar{R}(x,t) = R(x), \qquad \lim_{t\to\infty} \bar{S}(x,t) = a(x)t + b(x). \tag{14}$$

In the steady state

$$R(x+L) = R(x), \qquad a(x+L) = a(x), \qquad b(x+L) = b(x).$$

Combining (12), (13), (14), it can be verified that

$$\frac{\partial}{\partial x}\left[a(x)\frac{\partial \Phi}{\partial x} + k_B T\frac{\partial a(x)}{\partial x}\right] = 0, \tag{15}$$

$$\frac{\partial}{\partial x}\left[b(x)\frac{\partial \Phi}{\partial x} + k_B T\frac{\partial b(x)}{\partial x} - k_B T R(x)\right] + \xi J = \xi a(x), \tag{16}$$

where

$$J = -\frac{1}{\xi}\left(R\frac{\partial \Phi}{\partial x} + k_B T\frac{\partial R}{\partial x}\right). \tag{17}$$

At the steady state, (12) implies

$$\frac{\partial}{\partial x}\left(\frac{R}{\xi}\frac{\partial \Phi}{\partial x} + D\frac{\partial R}{\partial x}\right) = 0, \tag{18}$$

so $\partial J/\partial x = 0$, i.e. $J \equiv \text{const}$. Since $R(x)$ and $a(x)$ satisfy the same ordinary equation (12), (15), there exists a constant A such that

$$a(x) = AR(x). \tag{19}$$

From (16), (19), one can find

$$A = \int_0^L AR(x)\,dx = \int_0^L a(x)\,dx = \int_0^L J\,dx = JL =: \bar{V}, \tag{20}$$

i.e.

$$a(x) = \bar{V}R(x), \tag{21}$$

where $R(x)$ is one of the solutions of the ordinary equation (17) with periodic boundary condition $R(x) = R(x+L)$:

$$R(x) = -\frac{\xi J \exp\left(-\frac{\Phi(x)}{k_B T}\right)}{k_B T\left[\exp\left(\frac{\Delta\Phi}{k_B T}\right) - 1\right]}\left[\exp\left(\frac{\Delta\Phi}{k_B T}\right)\int_0^x \exp\left(\frac{\Phi(y)}{k_B T}\right)dy + \int_x^L \exp\left(\frac{\Phi(y)}{k_B T}\right)dy\right]$$
$$= -\frac{\xi J \exp\left(-\frac{\Phi(x)}{k_B T}\right)}{k_B T\left[\exp\left(\frac{\Delta\Phi}{k_B T}\right) - 1\right]}\int_x^{x+L} \exp\left(\frac{\Phi(y)}{k_B T}\right)dy, \tag{22}$$

and the constant J is determined by the normalization constraint $\int_0^L R(x)\,dx = 1$. The constant $\bar{V}$ in (21) is the mean velocity of Brownian particles. Actually, the mean velocity of the Brownian particles is

$$V := \lim_{t\to\infty} \frac{d}{dt} \int_{-\infty}^{\infty} x\rho(x,t)\,dx = \lim_{t\to\infty} \frac{d}{dt} \int_0^L \bar{S}(x,t)\,dx$$

$$= \lim_{t\to\infty} \int_0^L \frac{d}{dt} \bar{S}(x,t)\,dx = \int_0^L \frac{d}{dt}\big[a(x)t + b(x)\big]\,dx$$

$$= \int_0^L a(x)\,dx = \int_0^L J = JL = \bar{V}.$$

It can be easily found that, the formulation of the mean velocity $V = \bar{V}$ is the same as the one in [7].

2.2. The effective diffusion coefficient

In this subsection, we'll give the formulation of the effective diffusion coefficient. The effective diffusion coefficient is defined as

$$D_{\text{eff}} := \frac{1}{2} \lim_{t\to\infty} \left[\frac{d\overline{x^2}}{dt} - \frac{d(\bar{x})^2}{dt} \right], \tag{23}$$

where

$$\overline{x^k}(t) := \int_{-\infty}^{\infty} x^k \rho(x,t)\,dx, \quad k = 1, 2.$$

Due to Eq. (10)

$$\frac{d\overline{x^2}}{dt} = \int_{-\infty}^{\infty} x^2 \frac{\partial \rho(x,t)}{\partial t} dx = \frac{1}{\xi} \int_{-\infty}^{\infty} x^2 \frac{\partial}{\partial x}\left(\rho \frac{\partial \Phi}{\partial x} + k_B T \frac{\partial \rho}{\partial x} \right) dx$$

$$= -\frac{2}{\xi} \int_{-\infty}^{\infty} x\rho \frac{\partial \Phi}{\partial x} dx - 2D \int_{-\infty}^{\infty} x \frac{\partial \rho}{\partial x} dx$$

$$= -\frac{2}{\xi} \int_0^L \bar{S}(x,t) \frac{\partial \Phi}{\partial x} dx + 2D, \tag{24}$$

where $\rho(-\infty, t) = \rho(+\infty, t) = 0$ has been used. Therefore

$$\lim_{t\to\infty} \frac{d\overline{x^2}}{dt} = -\frac{2}{\xi} \int_0^L \big[a(x)t + b(x)\big] \frac{\partial \Phi}{\partial x} dx + 2D$$

$$= -\frac{2}{\xi} \int_0^L \big[JLR(x)t + b(x)\big] \frac{\partial \Phi}{\partial x} dx + 2D. \tag{25}$$

At the same time

$$\frac{d(\bar{x})^2}{dt} = 2\bar{x} \frac{d\bar{x}}{dt}$$

$$= 2\left(\int_{-\infty}^{\infty} x\rho\,dx \right)\left(\frac{d}{dt} \int_{\infty}^{\infty} x\rho\,dx \right)$$

$$= 2\left(\int_0^L \bar{S}\,dx \right)\left(\frac{d}{dt} \int_0^L \bar{S}\,dx \right) \tag{26}$$

by (14), (21), (26),

$$\lim_{t\to\infty} \frac{d(\bar{x})^2}{dt} = 2\left(\int_0^L \big(a(x)t + b(x)\big)\,dx \right)\left(\frac{d}{dt} \int_0^L \big(a(x)t + b(x)\big)\,dx \right)$$

$$= 2A\left[At + \int_0^L b(x)\,dx \right] = 2JL\left[JLt + \int_0^L b(x)\,dx \right]. \tag{27}$$

Combining (23), (24), (27), one obtains

$$D_{\text{eff}} = -\frac{1}{\xi} \int_0^L \left[\big(JLR(x)t + b(x)\big) \frac{\partial \Phi}{\partial x} \right] dx$$

$$- JL\left[JLt + \int_0^L b(x)\,dx \right] + D. \tag{28}$$

Due to (17)

$$-\frac{1}{\xi} \int_0^L R(x) \frac{\partial \Phi}{\partial x} dx = JL, \tag{29}$$

hence,

$$D_{\text{eff}} = -\frac{1}{\xi} \int_0^L b(x) \frac{\partial \Phi}{\partial x} dx - JL \int_0^L b(x)\,dx + D$$

$$= -\int_0^L b(x)\left[\frac{1}{\xi} \frac{\partial \Phi}{\partial x} + JL \right] dx + D. \tag{30}$$

The formulation of the effective diffusion coefficient D_{eff} can be obtained by (30) if the function $b(x)$ has been known. Thanks to (16), (19), the function $b(x)$ satisfies

$$k_B T \frac{\partial b}{\partial x} + \frac{\partial \Phi}{\partial x} b = \xi JL \int_0^x R(y)\,dy - \xi Jx + k_B T R(x) + C_1$$

$$\triangleq \Psi(x), \tag{31}$$

where C_1 is an arbitrary constant. So

$$b(x) = \exp\left(-\frac{\Phi(x)}{k_B T} \right)\left(\int_0^x \frac{\Psi(y)}{k_B T} \exp\left(\frac{\Phi(y)}{k_B T} \right) dy + C_2 \right) \tag{32}$$

and

$$\frac{1}{\xi} \int_0^L b(x) \frac{\partial \Phi}{\partial x} = \frac{1}{\xi} \int_0^L \Psi(x)\,dx - \frac{k_B T}{\xi} \int_0^L \frac{\partial b}{\partial x} dx = \frac{1}{\xi} \int_0^L \Psi(x)\,dx. \tag{33}$$

Combining (30), (32), (33)

$$D_{\text{eff}} = -\frac{1}{\xi} \int_0^L b(x) \frac{\partial \Phi}{\partial x} - JL \int_0^L b(x) + D$$

$$= -\frac{1}{\xi} \int_0^L \Psi(x)\,dx - JL \int_0^L b(x) + D$$

$$= -JL \int_0^L \int_0^x R(y)\,dy\,dx + \frac{1}{2} JL^2 - \frac{1}{\xi} C_1 L - JL \int_0^L b(x)\,dx. \tag{34}$$

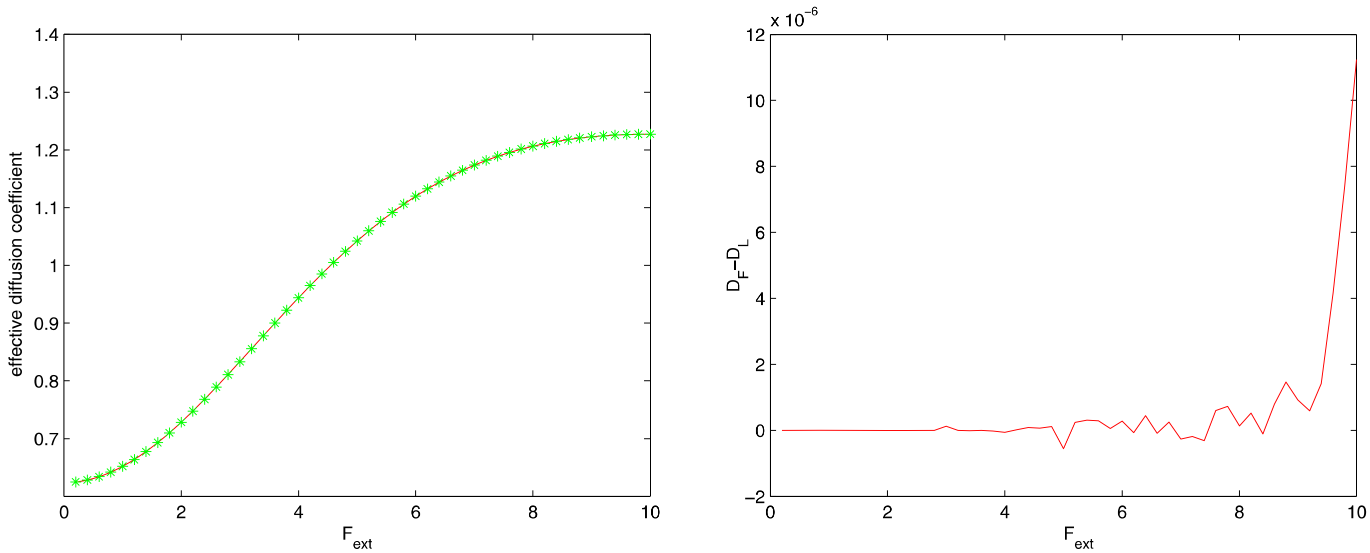

Fig. 1. Left: the relationship between the effective diffusion coefficient and the external force F_{ext}, where the red line is obtained by the formulation (41), the green stars are obtained by the formulation (2). Right: the difference between the formulation (41) and the formulation (2), where D_F denote the results of formulation (41), D_L denote the results of the formulation (2). In the simulation, the potential $\Phi(x) = U_0 \sin(2\pi x/L) - F_{\text{ext}}x$ and $\xi = U_0 = L = 1$ (see [8]). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this Letter.)

Remark. If $\frac{\partial \Phi}{\partial x} \equiv 0$ then $J = 0$, Eq. (30) implies $D_{\text{eff}} = D$. In the following, we assume $\Delta\Phi \neq 0$.

Since $b(0) = b(L)$, the solution of Eq. (31) is

$$\begin{aligned} b(x) &= \exp\left(-\frac{\Phi(x)}{k_B T}\right) \\ &\quad \times \left(\int_0^x \frac{\Psi(y)}{k_B T} \exp\left(\frac{\Phi(y)}{k_B T}\right) dy + \frac{\int_0^L \frac{\Psi(y)}{k_B T} \exp(\frac{\Phi(y)}{k_B T}) dy}{\exp(\frac{\Phi(L)-\Phi(0)}{k_B T}) - 1}\right) \\ &= \frac{\exp(-\frac{\Phi(x)}{k_B T})}{\exp(\frac{\Delta\Phi}{k_B T}) - 1}\left[\exp\left(\frac{\Delta\Phi}{k_B T}\right) \int_0^x \frac{\Psi(y)}{k_B T} \exp\left(\frac{\Phi(y)}{k_B T}\right) dy \right. \\ &\quad \left. + \int_x^L \frac{\Psi(y)}{k_B T} \exp\left(\frac{\Phi(y)}{k_B T}\right) dy\right]. \end{aligned} \tag{35}$$

Substituting the expression of function $\Psi(x)$ into (35), one obtains

$$b(x) = f(x) + C_1 g(x), \tag{36}$$

where

$$\begin{aligned} g(x) &= \frac{\exp(-\frac{\Phi(x)}{k_B T})}{k_B T[\exp(\frac{\Delta\Phi}{k_B T}) - 1]}\left[\exp\left(\frac{\Delta\Phi}{k_B T}\right) \int_0^x \exp\left(\frac{\Phi(y)}{k_B T}\right) dy \right. \\ &\quad \left. + \int_x^L \exp\left(\frac{\Phi(y)}{k_B T}\right) dy\right], \end{aligned} \tag{37}$$

$$f(x) = \frac{1}{\exp(\frac{\Delta\Phi}{k_B T}) - 1}\left[\exp\left(\frac{\Delta\Phi}{k_B T}\right) f_1(x) + f_2(x)\right], \tag{38}$$

$$\begin{aligned} f_1(x) &= -LR(x) \int_0^x R(z)\, dz \\ &\quad + \exp\left(-\frac{\Phi(x)}{k_B T}\right) \int_0^x R^2(z) \exp\left(\frac{\Phi(z)}{k_B T}\right) dz + R(x)x, \end{aligned}$$

$$\begin{aligned} f_2(x) &= LR(x) \int_0^x R(z)\, dz \\ &\quad + \exp\left(-\frac{\Phi(x)}{k_B T}\right) \int_x^L R^2(z) \exp\left(\frac{\Phi(z)}{k_B T}\right) dz - R(x)x. \end{aligned}$$

Eqs. (37), (22) imply

$$g(x) = -\frac{R(x)}{\xi J}. \tag{39}$$

Hence

$$\begin{aligned} D_{\text{eff}} &= -JL \int_0^L \int_0^x R(y)\, dy\, dx + \frac{1}{2} JL^2 - \frac{1}{\xi} C_1 L - JL \int_0^L b(x)\, dx \\ &= -JL \int_0^L \int_0^x R(y)\, dy\, dx + \frac{1}{2} JL^2 - JL \int_0^L f(x)\, dx. \end{aligned} \tag{40}$$

From (38) and (40), we finally get the formulation of the effective diffusion coefficient D_{eff}:

$$\begin{aligned} D_{\text{eff}} &= -JL \int_0^L \int_0^x R(y)\, dy\, dx \\ &\quad + \frac{1}{2} JL^2 + JL^2 \int_0^L R(x)\left(\int_0^x R(z)\, dz\right) dx - JL \int_0^L xR(x)\, dx \\ &\quad - \frac{JL}{\exp(\frac{\Delta\Phi}{k_B T}) - 1}\left\{\int_0^L \exp\left(-\frac{\Phi(x)}{k_B T}\right) \exp\left(\frac{\Delta\Phi}{k_B T}\right) \right. \\ &\quad \times \left[\int_0^x R^2(z) \exp\left(\frac{\Phi(z)}{k_B T}\right) dz\right] dx \end{aligned}$$

$$+\int_0^L \exp\left(-\frac{\Phi(x)}{k_BT}\right)\left[\int_x^L R^2(z)\exp\left(\frac{\Phi(z)}{k_BT}\right)dz\right]dx\Biggr\}$$

$$= J\int_0^L \left[\bigl(LR(x)-1\bigr)\int_0^x \bigl(LR(z)-1\bigr)\,dz\right]dx$$

$$-\frac{JL}{\exp(\frac{\Delta\Phi}{k_BT})-1}\int_0^L \exp\left(-\frac{\Phi(x)}{k_BT}\right)$$

$$\times\left[\int_x^{x+L} R^2(z)\exp\left(\frac{\Phi(z)}{k_BT}\right)dz\right]dx, \qquad (41)$$

in which J and $R(x)$ are given by Eq. (17) and Eq. (22), respectively.

3. Numerical results and conclusions

To demonstrate the accuracy of the formulation (41), we present the numerical results of the formulations (41) and (2) in Fig. 1. In fact, we have performed extensive computer simulations to demonstrate the accuracy of the formulation (41). There is practically no difference between the formulations (2) and (41).

In conclusion, in the framework of the Fokker–Planck equation and based on the moments of the particle's coordinate, the analytical expression of the effective diffusion coefficient D_{eff} of Brownian particles has been obtained in this research. As it is pointed out in the introduction, theoretically, our formulation (41) is not equivalent to the corresponding (2) which is obtained by P. Reimann et al., because different assumptions are used in their derivation. In our derivation, the assumption (14) means that, at steady state, the velocity of Brownian particle is periodic. However, the numerical comparison indicates that our analytical expression is also very accurate.

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