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EFFECTIVE DIFFUSION AND EFFECTIVE DRAG COEFFICIENT OF A BROWNIAN PARTICLE IN A PERIODIC POTENTIAL*

Dedicated to Professor Peter D. Lax on the occasion of his 85th birthday

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Abstract We study the stochastic motion of a Brownian particle driven by a constant force over a static periodic potential. We show that both the effective diffusion and the effective drag coefficient are mathematically well-defined and we derive analytic expressions for these two quantities. We then investigate the asymptotic behaviors of the effective diffusion and the effective drag coefficient, respectively, for small driving force and for large driving force. In the case of small driving force, the effective diffusion is reduced from its Brownian value by a factor that increases exponentially with the amplitude of the potential. The effective drag coefficient is increased by approximately the same factor. As a result, the Einstein relation between the diffusion coefficient and the drag coefficient is approximately valid when the driving force is small. For moderately large driving force, both the effective diffusion and the effective drag coefficient are increased from their Brownian values, and the Einstein relation breaks down. In the limit of very large driving force, both the effective diffusion and the effective drag coefficient converge to their Brownian values and the Einstein relation is once again valid.

Key words effective diffusion, effective drag coefficient, Einstein relation, Fokker-Planck equation, probability theory, asymptotic analysis

2000 MR Subject Classification 35QXX; 65CXX; 60JXX

1 Introduction and Mathematical Equations

We consider the one-diemnsional stochastic motion of a Brownian particle driven by a constant force over a static periodic potential. We are interested in the effective diffusion and the effective drag coefficient of the particle over long time. In single molecule experiments, the average velocity and the effective diffusion are the two important quantities that can be estimated from experimental data [1–4]. The effective drag coefficient is calculated directly from

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the measured average velocity. The effective diffusion is related to the randomness parameter, which reveals the internal mechanochemical details of a molecular motor [5, 6]. We like to know how the driving force and the static periodic potential affect the effective diffusion and the effective drag coefficient. This knowledge will be useful in deciphering the motor mechanism from experimental measurements in modeling studies of molecular motors [7–9].

As shown in Figure 1, a particle is driven by a constant force f over a static periodic potential $\phi(x)$ with period L. The combination of a constant force and a periodic potential can be viewed as a simplified model for protein motors [10, 11]. In addition to the driving force and the static potential, the particle is also subject to the Brownian diffusion caused by the bombardment of surrounding fluid molecules [12]. We consider the one-dimensional motion of the particle. Let $X(t)$ denote the stochastic position of the particle at time t. For a small particle in a viscous fluid environment, the inertia is negligible. Consequently, the dynamics of the particle is governed by the Langevin equation without inertia [13], which describes the balance of all forces on the particle:

$$0 = \underbrace{-\zeta\frac{\mathrm{d}X(t)}{\mathrm{d}t}}_{\text{Viscous drag}} \quad \underbrace{-\phi'(X)}_{\text{Force from potential}} \quad \underbrace{+f}_{\text{Driving force}} \quad \underbrace{+\sqrt{2k_BT\zeta}\,\frac{\mathrm{d}W(t)}{\mathrm{d}t}}_{\text{Brownian force}}. \tag{1}$$

In the above, ζ is the Brownian drag coefficient due to collisions between the particle and the surrounding fluid molecules, k_B is the Boltzmann constant and T is the absolute temperature [14, 15]. $W(t)$ is the standard Weiner process modeling the thermal Brownian motion [16].

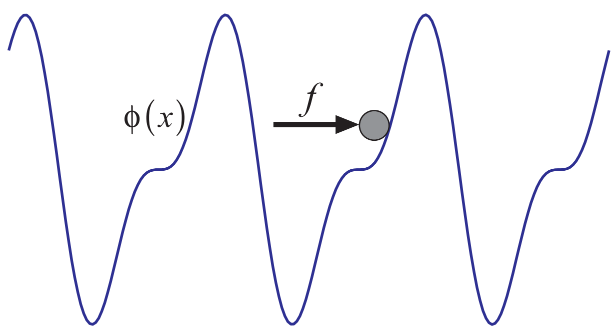

Fig.1 A particle driven by a constant force (f) over a static periodic potential ($\phi(x)$) and subject to the Brownian diffusion

Dividing (1) by ζ and expressing $\mathrm{d}X(t)/\mathrm{d}t$ in terms of others, we obtain the stochastic governing equation for $X(t)$:

$$\frac{\mathrm{d}X(t)}{\mathrm{d}t} = \frac{-\phi'(X)+f}{\zeta} + \sqrt{2D}\frac{\mathrm{d}W(t)}{\mathrm{d}t}, \tag{2}$$

where

$$D = \frac{k_BT}{\zeta} \tag{3}$$

is the Brownian diffusion coefficient. Equation (3) is called the Einstein relation [17], which relates the Brownian diffusion and the Brownian drag coefficient. The meaning of the Brownian diffusion can be seen by examining the simple case of $\phi'(x) \equiv 0$ (i.e., in the absence of a static periodic potential). In this case, the stochastic position of the particle is given by

$$X(t) = X(0) + \frac{f}{\zeta} \cdot t + \sqrt{2D}\, W(t).$$

The variance of particle position (in the absence of a potential) is

$$\mathrm{var}\,\{X(t)\} = 2D\,\mathrm{var}\,\{W(t)\} = 2D\,t.$$

Note that in the absence of a static periodic potential, the variance of particle position is always proportional to the time, for arbitrary time. As we will find out, in the presence of a static periodic potential, the variance of particle position is only asymptotically proportional to the time for long time.

In the presence of a static periodic potential, we define the average velocity and the effective diffusion coefficient of the particle as (the existence of the limits will be examined later)

$$V_{\mathrm{avg}} \equiv \lim_{t\to+\infty} \frac{\langle X(t)\rangle}{t},$$
$$D_{\mathrm{eff}} \equiv \lim_{t\to+\infty} \frac{\mathrm{var}\,\{X(t)\}}{2t}.$$

We define the effective drag coefficient as the effective resistance to the driving force

$$\zeta_{\mathrm{eff}} \equiv \frac{f}{V_{\mathrm{avg}}}.$$

In general, all these effective quantities vary with the driving force and the static periodic potential. So the full notation for the effective diffusion coefficient should be $D_{\mathrm{eff}}(f, [\phi])$. In the absence of a periodic potential, the effective diffusion coefficient is the same as the Brownian diffusion coefficient, which justifies the name of effective diffusion.

Since all average quantities can be calculated from the probability density, in this study, we derive the effective diffusion coefficient by following the time evolution of the probability density. Let $\rho(x,t)$ be the probability density that the particle is at position x at time t. Mathematically, $\rho(x,t)$ is defined as

$$\rho(x,t) \equiv \lim_{\Delta x\to 0+} \frac{\Pr\{x \le X(t) < x + \Delta x\}}{\Delta x}.$$

The time evolution of the probability density is governed by the Fokker-Planck equation [18] corresponding to Langevin equation (2):

$$\frac{\partial \rho}{\partial t} = D\frac{\partial}{\partial x}\left(\frac{\phi'(x) - f}{k_B T}\rho + \frac{\partial \rho}{\partial x}\right). \tag{4}$$

The probability density also satisfies the normalizing condition

$$\int_{-\infty}^{+\infty} \rho(x,t)\mathrm{d}x = 1.$$

To facilitate the analysis below, we non-dimensionalize all quantities. We introduce

$$\tilde{x} = \frac{x}{L}, \qquad \tilde{X} = \frac{X}{L}, \qquad \tilde{t} = \frac{t\,D}{L^2},$$
$$\tilde{\phi}(\tilde{x}) = \frac{\phi(x)}{k_B T}, \qquad \tilde{f} = \frac{f\,L}{k_B T},$$
$$\tilde{\rho}(\tilde{x},\tilde{t}) = L\,\rho(x,t).$$

It is straightforward to verify that $\tilde{\phi}(\tilde{x})$ is a periodic function with period 1 and that $\tilde{\rho}(\tilde{x},\tilde{t})$ satisfies the constraint $\int_{-\infty}^{+\infty}\rho(\tilde{x},\tilde{t})\mathrm{d}\tilde{x}=1$. In the derivation of the effective diffusion coefficient below, we will work only with the non-dimensionalized quantities. For the simplicity of presentation and without confusion, we drop the tildes in the rest of the paper and denote the non-dimensionalized quantities simply by $\{X, x, t, \phi, f, \rho, V_{\rm avg}, D_{\rm eff}, \zeta_{\rm eff}\}$. To distinguish dimensional and non-dimensional quantities, we denote the physical (dimensional) quantities by $\{X^{(p)}, x^{(p)}, t^{(p)}, \phi^{(p)}, f^{(p)}, \rho^{(p)}, V_{\rm avg}^{(p)}, D_{\rm eff}^{(p)}, \zeta_{\rm eff}^{(p)}\}$. For the non-dimensionalized variables, equation (4) becomes

$$\frac{\partial\rho}{\partial t}=\frac{\partial}{\partial x}\left(\left(\phi'(x)-f\right)\rho+\frac{\partial\rho}{\partial x}\right) \tag{5}$$

which, mathematically, corresponds to the special case of equation (4) with $L=1$, $D=1$, and $k_BT=1$. The dimensional and the non-dimensional $(V_{\rm avg}, D_{\rm eff}, \zeta_{\rm eff})$ are related by

$$\begin{aligned} V_{\rm avg}^{(p)} &= \frac{D}{L}\cdot V_{\rm avg},\\ \zeta_{\rm eff}^{(p)} &= \frac{k_BT}{D}\cdot\zeta_{\rm eff},\\ D_{\rm eff}^{(p)} &= D\cdot D_{\rm eff}. \end{aligned} \tag{6}$$

The non-dimensional $(V_{\rm avg}, D_{\rm eff}, \zeta_{\rm eff})$ has the expressions

$$\begin{aligned} V_{\rm avg} &\equiv \lim_{t\to+\infty}\frac{\langle X(t)\rangle}{t},\\ \zeta_{\rm eff} &\equiv \frac{f}{V_{\rm avg}},\\ D_{\rm eff} &\equiv \lim_{t\to+\infty}\frac{\left\langle X^2(t)\right\rangle-\langle X(t)\rangle^2}{2t}, \end{aligned} \tag{7}$$

where the j-th moment of the non-dimensional particle position is

$$\left\langle X^j(t)\right\rangle=\int_{-\infty}^{+\infty}x^j\rho(x,t)\mathrm{d}x. \tag{8}$$

In the absence of a static periodic potential ($\phi'(x)\equiv 0$), we have

$$(V_{\rm avg},\ D_{\rm eff},\ \zeta_{\rm eff})=(1,\ 1,\ 1).$$

The rest of the paper is organized as follows. In Section 2, we derive analytic expressions for the average velocity and the effective diffusion coefficient, based on governing equation (5) and definition (7). In Section 3, asymptotic analysis is carried out to investigate the trend of the effective diffusion and the effective drag coefficient in the regime of small driving force and in the regime of large driving force. The validity of the Einstein relation is also examined. In Section 4, the integral formulas derived in Section 2 are implemented numerically to compute the effective diffusion and the effective drag coefficient for arbitrary driving force. The numerical simulations will confirm the asymptotic results and will reveal the behaviors of the effective diffusion, the effective drag coefficient and the Einstein relation when the driving force is in the intermediate range. In Section 5, we discuss the results and observations.

2 Analytic Expressions for the Average Velocity and the Effective Diffusion Coefficient

In (8), the j-th moment of particle position $X(t)$ involves an integral over $(-\infty,+\infty)$. In differential equation (5), the potential $\phi(x)$ is periodic but the probability density $\rho(x,t)$ is not periodic in space. We like to exploit the fact that the driving force is constant and the static potential is periodic in space. Specifically, we like to express the j-th moment $\langle X^j(t)\rangle$ in terms of functions in $[0,1]$, instead of functions in $(-\infty,+\infty)$. Note that these moments are used in (7) to calculate the long time limits. Thus, we are allowed to use approximations for $\langle X^j(t)\rangle$ as long as the effect of errors disappears in the limit as $t\to+\infty$. We consider a coarse-graining representation of $X(t)$ defined as

$$N(t)\equiv\lfloor X(t)\rfloor, \tag{9}$$

where $\lfloor z\rfloor$ denotes the largest integer that is less than or equal to z. Note that $N(t)$ indicates which period the particle is in. Intuition tells us that over long time this coarse-graining representation is adequate for capturing the average velocity and the effective diffusion. The j-th moment of $N(t)$ is

$$\langle N^j(t)\rangle=\sum_{n=-\infty}^{+\infty}\int_n^{n+1}n^j\rho(x,t)\mathrm{d}x=\int_0^1\sum_{n=-\infty}^{+\infty}n^j\rho(n+x,t).$$

We introduce a sequence of functions:

$$\rho_j(x,t)\equiv\sum_{n=-\infty}^{+\infty}n^j\rho(n+x,t). \tag{10}$$

Function $\rho_0(x,t)$ is periodic:

$$\rho_0(x+1,t)=\rho_0(x,t).$$

$\rho_1(x,t)$ and $\rho_2(x,t)$ satisfy

$$\begin{aligned}\rho_1(x+1,t)&=\sum_{n=-\infty}^{+\infty}n\rho(n+x+1,t)=\sum_{n=-\infty}^{+\infty}(n-1)\rho(n+x,t)\\&=\rho_1(x,t)-\rho_0(x,t),\end{aligned}$$

$$\begin{aligned}\rho_2(x+1,t)&=\sum_{n=-\infty}^{+\infty}(n-1)^2\rho(n+x,t)\\&=\rho_2(x,t)-2\rho_1(x,t)+\rho_0(x,t).\end{aligned}$$

With function $\rho_j(x,t)$, the j-th moment of $N(t)$ is simply expressed as

$$\langle N^j(t)\rangle=\int_0^1\rho_j(x,t)\mathrm{d}x. \tag{11}$$

To relate the moments of $X(t)$ to those of $N(t)$, we re-write the j-th moment of $X(t)$ as

$$\begin{aligned}\langle X^j(t)\rangle&=\int_0^1\sum_{n=-\infty}^{+\infty}(n+x)^j\rho(n+x,t)\mathrm{d}x\\&=\int_0^1\sum_{n=-\infty}^{+\infty}n^j\rho(n+x,t)\mathrm{d}x+\int_0^1\sum_{n=-\infty}^{+\infty}\left((n+x)^j-n^j\right)\rho(n+x,t)\mathrm{d}x.\end{aligned}$$

Thus, the first two moments of $X(t)$ are expressed in terms of those of $N(t)$ as

$$\langle X(t)\rangle = \langle N(t)\rangle + \int_0^1 x\,\rho_0(x,t)\mathrm{d}x, \tag{12}$$

$$\left\langle X^2(t)\right\rangle = \left\langle N^2(t)\right\rangle + \int_0^1 2x\,\rho_1(x,t)\mathrm{d}x + \int_0^1 x^2\rho_0(x,t)\mathrm{d}x. \tag{13}$$

In the lemma below we show that $N(t)$ is indeed an adequate representation of $X(t)$ for the purpose of calculating the average velocity and the effective diffusion.

Lemma 1 If $\mathrm{var}\{N(t)\}$ satisfies $\mathrm{var}\{N(t)\} \le C\cdot t$ for large t, then the following is true:

$$\lim_{t\to\infty} \frac{\langle X(t)\rangle - \langle N(t)\rangle}{t} = 0, \tag{14}$$

$$\lim_{t\to\infty} \frac{\mathrm{var}\{X(t)\} - \mathrm{var}\{N(t)\}}{t} = 0. \tag{15}$$

Proof From definition (10), we see that $\rho_0(x,t)$ satisfies

$$\rho_0(x,t) > 0 \quad \text{and} \quad \int_0^1 \rho_0(x,t)\mathrm{d}x = 1.$$

Consequently, we have

$$0 < \int_0^1 x^j\rho_0(x,t)\mathrm{d}x < 1 \tag{16}$$

which, when combined with (12), leads directly to conclusion (14).

For the difference between variances, we use relations (12) and (13) to write $\mathrm{var}\{X(t)\} - \mathrm{var}\{N(t)\}$ as

$$\begin{aligned}\mathrm{var}\{X(t)\} - \mathrm{var}\{N(t)\} &= \left(\left\langle X^2(t)\right\rangle - \left\langle N^2(t)\right\rangle\right) - \left(\langle X(t)\rangle^2 - \langle N(t)\rangle^2\right)\\ &= \left(\int_0^1 2x\,\rho_1(x,t)\mathrm{d}x - 2\,\langle N(t)\rangle \int_0^1 x\,\rho_0(x,t)\mathrm{d}x\right)\\ &\quad + \left(\int_0^1 x^2\rho_0(x,t)\mathrm{d}x - \left(\int_0^1 x\,\rho_0(x,t)\mathrm{d}x\right)^2\right)\\ &\equiv I_1 + I_2.\end{aligned} \tag{17}$$

To prove (15), we only need to show

$$\lim_{t\to\infty} \frac{I_1 + I_2}{t} = 0.$$

With the help of (16), one can readily show $|I_2| < 1$. For I_1, we re-write it in the integral-summation form and then use the Cauchy-Schwarz inequality to derive

$$\begin{aligned}|I_1| &= 2\left|\int_0^1 x\cdot\left(\rho_1(x,t) - \langle N(t)\rangle\,\rho_0(x,t)\right)\mathrm{d}x\right|\\ &= 2\left|\int_0^1 \sum_{n=-\infty}^{\infty} x\cdot\left(n - \langle N(t)\rangle\right)\rho(n+x,t)\mathrm{d}x\right|\end{aligned}$$

$$
\begin{aligned}
&\le 2\sqrt{\int_0^1 \sum_{n=-\infty}^{\infty} x^2\rho(n+x,t)\mathrm{d}x \cdot \int_0^1 \sum_{n=-\infty}^{\infty} \left(n-\langle N(t)\rangle\right)^2 \rho(n+x,t)\mathrm{d}x} \\
&= 2\sqrt{\int_0^1 x^2\rho_0(x,t)\mathrm{d}x \cdot \mathrm{var}\{N(t)\}} \\
&\le 2\sqrt{C\cdot t}.
\end{aligned}
$$

It follows that $\lim_{t\to\infty}(I_1+I_2)/t=0$ and thus, conclusion (15) is true, which completes the proof of Lemma 1. □

Lemma 1 allows us to derive the average velocity and the effective diffusion coefficient using the moments of $N(t)$, which are conveniently expressed in terms of functions $\rho_j(x,t)$ in $[0,1]$:

$$
\begin{aligned}
&\lim_{t\to\infty}\frac{\langle X(t)\rangle}{t} = \lim_{t\to\infty}\frac{\langle N(t)\rangle}{t} = \lim_{t\to\infty}\frac{\int_0^1 \rho_1(x,t)\mathrm{d}x}{t}, \\
&\lim_{t\to\infty}\frac{\mathrm{var}\{X(t)\}}{2t} = \lim_{t\to\infty}\frac{\mathrm{var}\{N(t)\}}{2t} = \lim_{t\to\infty}\frac{\int_0^1 \rho_2(x,t)\mathrm{d}x - \left(\int_0^1 \rho_1(x,t)\mathrm{d}x\right)^2}{2t}.
\end{aligned}
$$

The meaning of the equations above is that if the limit on the right hand side exists then the limit on the left hand side also exists and is the same. To discuss the properties of $\rho_j(x,t)$, we introduce functions $w_0(x)$ and $w_1(x)$:

$$
w_0(x) \equiv \int_0^1 \exp(\phi(x+s)-\phi(x)-fs)\mathrm{d}s, \tag{18}
$$

$$
w_1(x) \equiv \int_0^1 w_0^2(x+s)\exp(\phi(x+s)-\phi(x)-fs)\mathrm{d}s. \tag{19}
$$

We start with the governing equation for $\rho_0(x,t)$. Since $\rho(x,t)$ satisfies (5), it is straightforward to verify that $\rho_0(x,t)$ satisfies (5) and the periodic boundary condition

$$
\frac{\partial \rho_0}{\partial t} = \frac{\partial}{\partial x}\left(\left(\phi'(x)-f\right)\rho_0 + \frac{\partial \rho_0}{\partial x}\right), \tag{20}
$$

$$
\rho_0(x+1,t)=\rho_0(x,t), \qquad \int_0^1 \rho_0(x,t)\mathrm{d}x = 1.
$$

Properties of $\rho_0(x,t)$ are described in the lemma below.

Lemma 2 As $t\to\infty$, function $\rho_0(x,t)$ converges to the steady state $u_0(x)$:

$$
\lim_{t\to\infty}\rho_0(x,t)=u_0(x), \tag{21}
$$

where the steady state $u_0(x)$ satisfies

$$
\left(\phi'(x)-f\right)u_0 + u_0' = -J_0 \tag{22}
$$

and is given by

$$
u_0(x) = \frac{J_0}{1-\mathrm{e}^{-f}}w_0(x), \qquad J_0 = \frac{1-\mathrm{e}^{-f}}{\int_0^1 w_0(x)\mathrm{d}x}. \tag{23}
$$

Proof Below we first derive the steady state $u_0(x)$ of (20). Then we show that $\rho_0(x,t)$ converges to the steady state $u_0(x)$ exponentially as $t\to\infty$. At the steady state, the probability flux is a constant J_0, independent of time and location. The steady state $u_0(x)$ of (20) satisfies

$$(\phi'(x)-f)\,u_0+u_0'=-J_0. \tag{24}$$

Multiplying by the integration factor and integrating from x to $x+1$, we get

$$\exp(\phi(s)-fs)u_0(s)|_x^{x+1}=-J_0\int_x^{x+1}\exp(\phi(s)-fs)\mathrm{d}s.$$

Applying the periodic condition $u_0(x+1)=u_0(x)$ yields

$$u_0(x)=\frac{J_0}{1-\mathrm{e}^{-f}}\exp(-\phi(x)+fx)\int_x^{x+1}\exp(\phi(s)-fs)\mathrm{d}s.$$

Making a change of variable $s_{\rm old}=x+s_{\rm new}$, we obtain

$$u_0(x)=\frac{J_0}{1-\mathrm{e}^{-f}}w_0(x),$$

where $w_0(x)$ is defined in (18). The expression for J_0 stated in (23) follows directly from the condition $\int_0^1 u_0(x)\mathrm{d}x=1$.

To complete the proof, it remains to show that $\lim\limits_{t\to\infty}\rho_0(x,t)=u_0(x)$. We consider function

$$r_0(x,t)=\frac{\rho_0(x,t)-u_0(x)}{u_0(x)}. \tag{25}$$

We only need to show $\lim\limits_{t\to\infty}r_0(x,t)=0$. Both $\rho_0(x,t)$ and $u_0(x)$ satisfy linear differential equation (20). As a result, the difference $\rho_0(x,t)-u_0(x)=u_0(x)r_0(x,t)$ satisfies equation (20). Substituting $u_0(x)r_0(x,t)$ into equation (20) and using (24), we obtain a differential equation for $r_0(x,t)$ with the periodic boundary condition:

$$u_0\frac{\partial r_0}{\partial t}=\frac{\partial}{\partial x}\left(-J_0r_0+u_0\frac{\partial r_0}{\partial x}\right), \tag{26}$$

$$r_0(x+1,t)=r_0(x,t),\qquad \int_0^1 u_0(x)r_0(x,t)\mathrm{d}x=0.$$

Note that in differential equation (26), J_0 is a constant, independent of (x,t). We study the time evolution of quantity $\int_0^1 u_0(x)r_0^2(x,t)\mathrm{d}x$. Since $u_0(x)$ is positive and is independent of t, we only need to show $\lim\limits_{t\to\infty}\int_0^1 u_0(x)r_0^2(x,t)\mathrm{d}x=0$. Using the differential equation and integration by parts, and then applying the periodic boundary condition, we derive

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_0^1 u_0r_0^2\mathrm{d}x&=2\int_0^1 u_0r_0\frac{\partial r_0}{\partial t}\mathrm{d}x\\ &=2\int_0^1 r_0\frac{\partial}{\partial x}\left(-J_0r_0+u_0\frac{\partial r_0}{\partial x}\right)\mathrm{d}x\\ &=-\int_0^1 J_0\frac{\partial r_0^2}{\partial x}-2\int_0^1 u_0\left(\frac{\partial r_0}{\partial x}\right)^2\mathrm{d}x\\ &=-2\int_0^1 u_0\left(\frac{\partial r_0}{\partial x}\right)^2\mathrm{d}x\le 0.\end{aligned} \tag{27}$$

We like to show that $\int_0^1 u_0 r_0^2 \mathrm{d}x$ decays exponentially to zero. For that purpose, we only need to show

$$\int_0^1 u_0 r_0^2 \mathrm{d}x \le C \int_0^1 u_0 \left(\frac{\partial r_0}{\partial x}\right)^2 \mathrm{d}x.$$

Integrating $\partial r_0/\partial x$ from y to z gives us

$$r_0(z,t) = r_0(y,t) + \int_y^z \frac{\partial r_0}{\partial x}\mathrm{d}x.$$

Multiplying by $u_0(y)$, integrating with respect to y from 0 to 1, and using $\int_0^1 u_0(y)\mathrm{d}y = 1$ and $\int_0^1 u_0(y) r_0(y,t)\mathrm{d}y = 0$, we get

$$r_0(z,t) = \int_0^1 u_0(y) \int_y^z \frac{\partial r_0}{\partial x}\mathrm{d}x\mathrm{d}y.$$

For $z \in [0,1]$, taking the absolute value and using the Cauchy-Schwarz inequality yields

$$\begin{aligned} |r_0(z,t)| &\le \int_0^1 u_0(y) \left|\int_y^z \frac{\partial r_0}{\partial x}\mathrm{d}x\right| \mathrm{d}y \le \int_0^1 u_0(y) \int_0^1 \left|\frac{\partial r_0}{\partial x}\right| \mathrm{d}x\mathrm{d}y \\ &= \int_0^1 \left|\frac{\partial r_0}{\partial x}\right| \mathrm{d}x \le \sqrt{\int_0^1 \left(\frac{\partial r_0}{\partial x}\right)^2 \mathrm{d}x}. \end{aligned}$$

The inequality above is valid for any $z \in [0,1]$. $\int_0^1 u_0 r_0^2 \mathrm{d}x$ is bounded by

$$\begin{aligned} \int_0^1 u_0 r_0^2 \mathrm{d}x &\le \max_x r_0^2(x,t) \int_0^1 u_0(x)\mathrm{d}x \le \int_0^1 \left(\frac{\partial r_0}{\partial x}\right)^2 \mathrm{d}x \\ &\le \frac{1}{\min\limits_x u_0(x)} \int_0^1 u_0 \left(\frac{\partial r_0}{\partial x}\right)^2 \mathrm{d}x. \end{aligned} \tag{28}$$

Combining (27) and (28), we arrive at

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_0^1 u_0 r_0^2 \mathrm{d}x \le -2 \min_x u_0(x) \cdot \int_0^1 u_0 r_0^2 \mathrm{d}x.$$

From this differential inequality, we can derive

$$\int_0^1 u_0(x) r_0^2(x,t)\mathrm{d}x \le C \cdot \exp\left(-t \cdot 2 \min_x u_0(x)\right),$$

which implies $\lim\limits_{t\to\infty} r_0(x,t) = 0$. Therefore, we conclude $\lim\limits_{t\to\infty} \rho_0(x,t) = u_0(x)$. This completes the proof of Lemma 2. □

Lemma 2 shows that $\rho_0(x,t)$ converges to $u_0(x)$ exponentially as $t \to \infty$. Without loss of generality, we assume that $\rho_0(x,t)$ is already at the steady state at $t = 0$. Specifically, we set the initial probability density of particle position as

$$\rho(x,0) = \begin{cases} u_0(x), & 0 \le x \le 1, \\ 0, & \text{otherwise.} \end{cases}$$

With this initial probability density, we have

$$\rho_0(x,t) = u_0(x), \qquad \text{for all } t,$$

$$\rho_1(x,0) = \sum_{n=-\infty}^{+\infty} n\,\rho(n+x,0) = 0, \qquad \text{for } 0 \le x \le 1.$$

Next we look at the governing equation for $\rho_1(x,t)$. From the definition of $\rho_1(x,t)$, we can verify that $\rho_1(x,t)$ satisfies (5) with the initial and boundary conditions below:

$$\frac{\partial \rho_1}{\partial t} = \frac{\partial}{\partial x}\left((\phi'(x) - f)\,\rho_1 + \frac{\partial \rho_1}{\partial x} \right), \tag{29}$$
$$\rho_1(x+1,t) = \rho_1(x,t) - u_0(x),$$
$$\rho_1(x,0) = 0, \qquad \text{for } x \in [0,1].$$

Before solving for $\rho_1(x,t)$, we use the differential equation and the boundary condition of $\rho_1(x,t)$ to write out the average velocity:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle N(t)\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^1 \rho_1(x,t)\mathrm{d}x = \int_0^1 \frac{\partial}{\partial t}\rho_1(x,t)\mathrm{d}x \\
&= \int_0^1 \frac{\partial}{\partial x}\left((\phi'(x) - f)\,\rho_1 + \frac{\partial \rho_1}{\partial x} \right)\mathrm{d}x \\
&= \left((\phi'(x) - f)\,\rho_1 + \frac{\partial \rho_1}{\partial x} \right)\Big|_0^1 \\
&= -\left((\phi'(x) - f)\,u_0 + u_0' \right)\big|_0 = J_0,
\end{aligned}$$

where the steady state flux J_0 is given in (23). The initial condition $\rho_1(x,0) = 0$ gives us $\langle N(0)\rangle = 0$. Thus, we have $\langle N(t)\rangle = J_0\,t$ and the average velocity has the expression

$$V_{\rm avg} = \lim_{t\to\infty}\frac{\langle N(t)\rangle}{t} = \lim_{t\to\infty}\frac{\mathrm{d}}{\mathrm{d}t}\langle N(t)\rangle = J_0 = \frac{1 - \mathrm{e}^{-f}}{\int_0^1 w_0(x)\mathrm{d}x}. \tag{30}$$

When the driving force (f) is non-zero, $\langle N(t)\rangle = \int_0^1 \rho_1(x,t)\mathrm{d}x$ increases linearly with t. It is clear that we should not expect $\rho_1(x,t)$ to reach a steady state as $t \to \infty$. Instead, we consider function

$$p_1(x,t) \equiv \rho_1(x,t) - J_0\,t\,u_0(x). \tag{31}$$

Here the coefficient $J_0\,t$ is selected to make $\int_0^1 p_1(x,t) = 0$ so it is possible for $p_1(x,t)$ to converge to a steady state. The governing differential equation for $p_1(x,t)$ can be derived by substituting $\rho_1(x,t) = p_1(x,t) + J_0\,t\,u_0(x)$ into equation (29):

$$\frac{\partial p_1}{\partial t} + J_0 u_0 = \frac{\partial}{\partial x}\left((\phi'(x) - f)\,p_1 + \frac{\partial p_1}{\partial x} \right), \tag{32}$$

$$p_1(x+1,t) = p_1(x,t) - u_0(x), \qquad \int_0^1 p_1(x,t) = 0.$$

The lemma below contains the results for $p_1(x,t)$.

Lemma 3 As $t \to \infty$, function $p_1(x,t)$ converges to the steady state $u_1(x)$:

$$\lim_{t\to\infty} p_1(x,t) = u_1(x). \tag{33}$$

The steady state $u_1(x)$ satisfies

$$(\phi'(x) - f)\, u_1 + u_1' = -J_1 + J_0 \int_0^x u_0(s)\mathrm{d}s, \tag{34}$$

and has the expression

$$u_1(x) = u_0(x)\left(\frac{J_1}{J_0} - \int_0^x u_0(s)\mathrm{d}s\right) - \frac{w_1(x)}{J_0\left(\int_0^1 w_0(x)\mathrm{d}x\right)^3}, \tag{35}$$

where the constant J_1 is given by

$$J_1 = \frac{\int_0^1 w_1(x)\mathrm{d}x}{\left(\int_0^1 w_0(x)\mathrm{d}x\right)^3} + \frac{J_0}{2}. \tag{36}$$

Proof Similar to what we did in the proof of Lemma 2, below we first derive the steady state $u_1(x)$ of (32). Then we show that $p_1(x,t)$ converges to the steady state $u_1(x)$ exponentially as $t \to \infty$. The steady state $u_1(x)$ satisfies

$$J_0\, u_0 = \frac{\mathrm{d}}{\mathrm{d}x}\left((\phi'(x) - f)\, u_1 + u_1'\right).$$

Integrating both sides yields

$$(\phi'(x) - f)\, u_1 + u_1' = -J_1 + J_0 \int_0^x u_0(s)\mathrm{d}s,$$

where J_1 is the integration constant, to be determined in the calculation below. Multiplying by the integration factor and integrating from x to $x+1$, we have

$$\exp(\phi(s) - fs)u_1(s)\big|_x^{x+1} = \int_x^{x+1} \exp(\phi(s) - fs)\left(-J_1 + J_0\int_0^s u_0(y)\mathrm{d}y\right)\mathrm{d}s. \tag{37}$$

Recall that in Lemma 2 when we multiply the differential equation (24) for u_0 by the integration factor, we can derive

$$\exp(\phi(s) - fs) = \frac{-1}{J_0}\cdot\frac{\mathrm{d}}{\mathrm{d}s}\left(\exp(\phi(s) - fs)u_0(s)\right).$$

Substituting this result into the right hand side (RHS) of (37), carrying out integration by parts and using $\int_x^{x+1} u_0(y)\mathrm{d}y = 1$, and for the left hand side (LHS) of (37), applying the boundary condition $u_1(x+1) = u_1(x) - u_0(x)$, we get

$$\mathrm{LHS} = \exp(\phi(x) - fx)\left[(\mathrm{e}^{-f} - 1)u_1(x) - \mathrm{e}^{-f}u_0(x)\right],$$

$$\begin{aligned}\mathrm{RHS} = {}&\frac{-1}{J_0}\exp(\phi(x) - fx)u_0(x)\left[(\mathrm{e}^{-f} - 1)\left(-J_1 + J_0\int_0^x u_0(y)\mathrm{d}y\right) + \mathrm{e}^{-f}J_0\right]\\ &+\int_x^{x+1}\exp(\phi(s) - fs)u_0^2(s)\mathrm{d}s.\end{aligned}$$

Using the expression of $u_0(x)$ that we derived in Lemma 2 and applying change of variable $s_{\text{old}} = x + s_{\text{new}}$, we write the last term of the RHS in terms of function $w_1(x)$:

$$\begin{aligned}
&\int_x^{x+1} \exp(\phi(s) - fs)u_0^2(s)\mathrm{d}s \\
= &\frac{1}{\left(\int_0^1 w_0(s)\mathrm{d}s\right)^2} \int_x^{x+1} \exp(\phi(s) - fs)w_0^2(s)\mathrm{d}s \\
= &\frac{\exp(\phi(x) - fx)}{\left(\int_0^1 w_0(s)\mathrm{d}s\right)^2} \int_0^1 \exp(\phi(x+s) - \phi(x) - fs)w_0^2(x+s)\mathrm{d}s \\
= &\frac{\exp(\phi(x) - fx)(1 - \mathrm{e}^{-f})}{J_0\left(\int_0^1 w_0(s)\mathrm{d}s\right)^3} w_1(x),
\end{aligned} \tag{38}$$

where $w_1(x)$ is defined in (19). Setting LHS = RHS and solving for $u_1(x)$ from it leads us to the expression of $u_1(x)$ stated in (35):

$$u_1(x) = u_0(x)\left(\frac{J_1}{J_0} - \int_0^x u_0(s)\mathrm{d}s\right) - \frac{w_1(x)}{J_0\left(\int_0^1 w_0(s)\mathrm{d}s\right)^3}.$$

The expression of J_1 is derived from the constraint $\int_0^1 u_1(x)\mathrm{d}x = 0$. Integrating the equation above, and using $\int_0^1 u_0(x)\mathrm{d}x = 1$ and $\int_0^1 u_0(x)\int_0^x u_0(s)\mathrm{d}s = \frac{1}{2}\left(\int_0^1 u_0(s)\mathrm{d}s\right)^2 = \frac{1}{2}$, we obtain

$$\frac{J_1}{J_0} - \frac{1}{2} - \frac{\int_0^1 w_1(x)\mathrm{d}x}{J_0\left(\int_0^1 w_0(s)\mathrm{d}s\right)^3} = 0,$$

which implies (36).

The second part of the proof is to show that $\lim\limits_{t\to\infty} p_1(x,t) = u_1(x)$. We consider function

$$r_1(x,t) = \frac{p_1(x,t) - u_1(x)}{u_0(x)}. \tag{39}$$

We only need to show $\lim\limits_{t\to\infty} r_1(x,t) = 0$. Both $p_1(x,t)$ and $u_1(x)$ satisfy linear differential equation (32). Consequently, the difference $p_1(x,t) - u_1(x) = u_0(x)r_1(x,t)$ satisfies equation (32). Substituting $u_0(x)r_1(x,t)$ into equation (32) and using (22), we obtain a differential equation for $r_1(x,t)$ with the periodic boundary condition:

$$u_0\frac{\partial r_1}{\partial t} = \frac{\partial}{\partial x}\left(-J_0 r_1 + u_0\frac{\partial r_1}{\partial x}\right), \tag{40}$$

$$r_1(x+1,t) = r_1(x,t), \qquad \int_0^1 u_0(x)r_1(x,t)\mathrm{d}x = 0.$$

Notice that system (40) is exactly the same as system (26). Using the same method as we employed in the proof of Lemma 2, we can show that $\int_0^1 u_0(x)r_1^2(x,t)\mathrm{d}x$ decays exponentially to zero as $t \to \infty$. Thus, we conclude that $\lim\limits_{t\to\infty} p_1(x,t) = u_1(x)$, which completes the proof of Lemma 3. □

In order to calculate the effective diffusion, we need to know the governing equation for $\rho_2(x,t)$. From the definition of $\rho_2(x,t)$, we can verify that $\rho_2(x,t)$ satisfies (5) with the initial and boundary conditions below:

$$\begin{aligned}
&\frac{\partial \rho_2}{\partial t} = \frac{\partial}{\partial x}\left(\left(\phi'(x) - f\right)\rho_2 + \frac{\partial \rho_2}{\partial x}\right), \\
&\rho_2(x+1,t) = \rho_2(x,t) - 2\rho_1(x,t) + u_0(x), \\
&\rho_2(x,0) = 0, \qquad \text{for } x \in [0,1].
\end{aligned} \tag{41}$$

Using this differential equation, we write the derivative of $\langle N^2(t)\rangle$ as

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle N^2(t)\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^1 \rho_2(x,t)\mathrm{d}x = \int_0^1 \frac{\partial}{\partial t}\rho_2(x,t)\mathrm{d}x \\
&= \int_0^1 \frac{\partial}{\partial x}\left(\left(\phi'(x) - f\right)\rho_2 + \frac{\partial \rho_2}{\partial x}\right)\mathrm{d}x \\
&= \left(\left(\phi'(x) - f\right)\rho_2 + \frac{\partial \rho_2}{\partial x}\right)\Bigg|_0^1.
\end{aligned}$$

After we apply the boundary condition $\rho_2(x+1,t) = \rho_2(x,t) - 2\rho_1(x,t) + u_0(x)$, the relation $\rho_1(x,t) = p_1(x,t) + J_0\, t\, u_0(x)$, and the result $((\phi'(x) - f)\, u_0 + u_0') = -J_0$, the derivative of $\langle N^2(t)\rangle$ takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle N^2(t)\rangle = -2\left(\left(\phi'(x) - f\right)p_1 + \frac{\partial p_1}{\partial x}\right)\Bigg|_0 + (2J_0\, t - 1)J_0.$$

For calculating the effective diffusion, we need to study the derivative of $\mathrm{var}\,\{N(t)\}$. Recall that after Lemma 2 we have derived $\langle N(t)\rangle = J_0\, t$. We write the derivative of $\mathrm{var}\,\{N(t)\}$ as

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{var}\,\{N(t)\} &= \frac{\mathrm{d}}{\mathrm{d}t}\langle N^2(t)\rangle - \frac{\mathrm{d}}{\mathrm{d}t}\langle N(t)\rangle^2 \\
&= -2\left(\left(\phi'(x) - f\right)p_1 + \frac{\partial p_1}{\partial x}\right)\Bigg|_0 - J_0.
\end{aligned}$$

Taking the limit as $t \to \infty$, using the results (which we have proved in Lemma 3)

$$\begin{aligned}
&\lim_{t\to\infty} p_1(x,t) = u_1(x), \\
&((\phi'(x) - f)\, u_1 + u_1') = -J_1 + J_0\int_0^x u_0(s)\mathrm{d}s,
\end{aligned}$$

and using the expression of J_1 given in (36), we finally arrive at

$$\begin{aligned}
D_{\text{eff}} &= \lim_{t\to\infty}\frac{\mathrm{var}\,\{N(t)\}}{2t} = \frac{1}{2}\lim_{t\to\infty}\frac{\mathrm{d}}{dt}\mathrm{var}\,\{N(t)\} \\
&= J_1 - \frac{J_0}{2} = \frac{\int_0^1 w_1(x)\mathrm{d}x}{\left(\int_0^1 w_0(x)\mathrm{d}x\right)^3}.
\end{aligned} \tag{42}$$

The main theorem below summarizes the integral expressions we derived for V_{avg} and D_{eff}.

Theorem Consider the non-dimensionalized case of a Brownian particle with Brownian diffusion coefficient $= 1$, driven by a constant force (f) over a static periodic potential $(\phi(x))$

with period = 1. The average velocity, the effective diffusion and the effective drag coefficient are well defined (that is, the limits in their definitions exist) and they are given by

$$V_{\text{avg}} \equiv \lim_{t\to\infty} \frac{\langle N(t)\rangle}{t} = \frac{1-\mathrm{e}^{-f}}{\int_0^1 w_0(s)\mathrm{d}s}, \tag{43}$$

$$D_{\text{eff}} \equiv \lim_{t\to\infty} \frac{\text{var}\{N(t)\}}{2t} = \frac{\int_0^1 w_1(s)\mathrm{d}s}{\left(\int_0^1 w_0(s)\mathrm{d}s\right)^3}, \tag{44}$$

$$\zeta_{\text{eff}} \equiv \frac{f}{V_{\text{avg}}} = \frac{f}{1-\mathrm{e}^{-f}} \int_0^1 w_0(s)\mathrm{d}s, \tag{45}$$

where functions $w_0(x)$ and $w_1(x)$ are defined as

$$w_0(x) \equiv \int_0^1 \exp(\phi(x+s)-\phi(x)-fs)\mathrm{d}s, \tag{46}$$

$$w_1(x) \equiv \int_0^1 w_0^2(x+s)\exp(\phi(x+s)-\phi(x)-fs)\mathrm{d}s. \tag{47}$$

3 Asymptotic Behaviors of the Effective Diffusion and the Effective Drag Coefficient

We study the asymptotic behaviors of the effective diffusion and the effective drag coefficient in two regimes: 1) small driving force and 2) large driving force.

Regime 1 f is small.

When the driving force (f) is small, we expand everything with respect to f:

$$1-\mathrm{e}^{-f} = f\left[1-\frac{f}{2}+O\left(f^2\right)\right],$$

$$\frac{f}{1-\mathrm{e}^{-f}} = 1+\frac{f}{2}+O\left(f^2\right),$$

$$w_0(x) = \mathrm{e}^{-\phi(x)}\left[\int_0^1 \mathrm{e}^{\phi(x+s)}\mathrm{d}s - f\int_0^1 \mathrm{e}^{\phi(x+s)}s\,\mathrm{d}s + O\left(f^2\right)\right].$$

Recall a useful property of periodic functions: if $g(s)$ is periodic with period = 1, then

$$\int_x^{x+1} g(s)\mathrm{d}s = \int_0^1 g(s)\mathrm{d}s. \tag{48}$$

Applying this property in calculating $\int_0^1 w_0(x)\mathrm{d}x$, we get

$$\int_0^1 w_0(x)\mathrm{d}x = a_0\left[1-f\frac{a_1}{a_0}+O\left(f^2\right)\right],$$

where coefficients a_0 and a_1 are given by

$$a_0 = \left(\int_0^1 \mathrm{e}^{\phi(s)}\mathrm{d}s\right)\left(\int_0^1 \mathrm{e}^{-\phi(s)}\mathrm{d}s\right), \tag{49}$$

$$a_1 = \int_0^1\int_0^1 \mathrm{e}^{\phi(x+s)-\phi(x)}\,s\,\mathrm{d}s\,\mathrm{d}x. \tag{50}$$

To calculate $\int_0^1 w_1(x)\mathrm{d}x$, we use property (48) to re-write it as

$$\begin{aligned}\int_0^1 w_1(x)\mathrm{d}x &= \int_0^1\int_0^1 w_0^2(x+s)\mathrm{e}^{\phi(x+s)-\phi(x)-fs}\,\mathrm{d}x\mathrm{d}s\\ &= \int_0^1\int_0^1 w_0^2(x)\mathrm{e}^{\phi(x)-\phi(x-s)-fs}\,\mathrm{d}x\mathrm{d}s\\ &= \int_0^1 w_0^2(x)\mathrm{e}^{\phi(x)}\left[\int_0^1 \mathrm{e}^{-\phi(s)}\mathrm{d}s - f\int_0^1 \mathrm{e}^{-\phi(x-s)}\,s\,\mathrm{d}s + O\left(f^2\right)\right]\mathrm{d}x.\end{aligned}$$

Substituting into it the expansion of $w_0(x)$ and using change of variable $s_{\text{old}} = 1 - s_{\text{new}}$ on the term below

$$\begin{aligned}I_3 &\equiv \int_0^1\int_0^1 \mathrm{e}^{-\phi(x)}\mathrm{e}^{-\phi(x-s)}\,s\,\mathrm{d}s\,\mathrm{d}x\\ &= \int_0^1\int_0^1 \mathrm{e}^{-\phi(x)}\mathrm{e}^{-\phi(x+s)}\,(1-s)\,\mathrm{d}s\,\mathrm{d}x\\ &= \int_0^1\int_0^1 \mathrm{e}^{-\phi(x-s)}\mathrm{e}^{-\phi(x)}\,(1-s)\,\mathrm{d}s\,\mathrm{d}x\\ &= \int_0^1\int_0^1 \mathrm{e}^{-\phi(x-s)}\mathrm{e}^{-\phi(x)}\,\mathrm{d}s\,\mathrm{d}x - I_3\\ &= a_0^2 - I_3,\end{aligned}$$

we obtain

$$\begin{aligned}\int_0^1 w_1(x)\mathrm{d}x &= \int_0^1 \mathrm{e}^{-\phi(x)}\left[\left(\int_0^1 \mathrm{e}^{\phi(s)}\mathrm{d}s\right)^2 - 2f\int_0^1 \mathrm{e}^{\phi(s)}\mathrm{d}s\int_0^1 \mathrm{e}^{\phi(x+s)}\,s\,\mathrm{d}s + O\left(f^2\right)\right]\\ &\quad\times\left[\int_0^1 \mathrm{e}^{-\phi(s)}\mathrm{d}s - f\int_0^1 \mathrm{e}^{-\phi(x-s)}\,s\,\mathrm{d}s + O\left(f^2\right)\right]\mathrm{d}x\\ &= a_0^2 - f\left(2a_0a_1 + \frac{1}{2}a_0^2\right) + O\left(f^2\right)\\ &= a_0^2\left[1 - f\left(\frac{2a_1}{a_0} + \frac{1}{2}\right) + O\left(f^2\right)\right].\end{aligned}$$

The effective drag coefficient and the effective diffusion have the expansions:

$$V_{\text{avg}} = \frac{1-\mathrm{e}^{-f}}{\int_0^1 w_0(x)\mathrm{d}x} = \frac{f}{a_0}\left[1 + f\cdot\frac{2a_1 - a_0}{2a_0} + O\left(f^2\right)\right], \tag{51}$$

$$\zeta_{\text{eff}} = \frac{f\int_0^1 w_0(x)\mathrm{d}x}{1-\mathrm{e}^{-f}} = a_0\left[1 - f\cdot\frac{2a_1 - a_0}{2a_0} + O\left(f^2\right)\right], \tag{52}$$

$$D_{\text{eff}} = \frac{\int_0^1 w_1(x)\mathrm{d}x}{\left(\int_0^1 w_0(x)\mathrm{d}x\right)^3} = \frac{1}{a_0}\left[1 + f\cdot\frac{2a_1 - a_0}{2a_0} + O\left(f^2\right)\right]. \tag{53}$$

The non-dimensional version of the Einstein relation is

$$\text{Drag coefficient} \times \text{Diffusion coefficient} = 1.$$

For small driving force, the Einstein relation is valid up to the $O(f)$ term

$$\zeta_{\text{eff}} \cdot D_{\text{eff}} = 1 + O\left(f^2\right).$$

When the driving force is small, the leading term of the effective diffusion is $D_{\text{eff}} = 1/a_0$. The Cauchy-Schwarz inequality guarantees that $a_0 \geq 1$:

$$a_0 = \left(\int_0^1 \mathrm{e}^{-\phi(s)}\mathrm{d}s\right)\left(\int_0^1 \mathrm{e}^{+\phi(s)}\mathrm{d}s\right) \geq \left(\int_0^1 \sqrt{\mathrm{e}^{-\phi(s)}}\cdot\sqrt{\mathrm{e}^{+\phi(s)}}\,\mathrm{d}s\right)^2 = 1.$$

Coefficient a_0 increases roughly exponentially with the amplitude of the potential. To demonstrate the exponential growth, we consider the special case of $\phi(x) = \alpha(2x-1)^2$. For this potential, coefficient a_0 can be expressed as

$$\begin{aligned} a_0 &= \left(\int_0^1 \mathrm{e}^{-\alpha(2s-1)^2}\mathrm{d}s\right)\left(\int_0^1 \mathrm{e}^{+\alpha(2s-1)^2}\mathrm{d}s\right) \\ &= \left(\frac{\sqrt{\pi}}{2\sqrt{\alpha}}\cdot \operatorname{erf}(\sqrt{\alpha})\right)\left(\frac{\mathrm{e}^{\alpha}}{\sqrt{\alpha}}\cdot F_{\text{Dawson}}(\sqrt{\alpha})\right), \end{aligned}$$

where $\operatorname{erf}(z) \equiv \frac{2}{\sqrt{\pi}}\int_0^z \mathrm{e}^{-s^2}\mathrm{d}s$ is the Gauss error function and $F_{\text{Dawson}}(z) \equiv \mathrm{e}^{-z^2}\int_0^z \mathrm{e}^{+s^2}\mathrm{d}s$ is the Dawson's function. For large z, they have the asymptotic behaviors:

$$\operatorname{erf}(z) \approx 1, \qquad F_{\text{Dawson}}(z) \approx \frac{1}{2z}.$$

For large α, the coefficient a_0 is approximately

$$a_0 \approx \frac{\sqrt{\pi}}{4\alpha^{3/2}}\mathrm{e}^{\alpha},$$

which increases exponentially with α. Thus, when the amplitude of the potential is moderately large and driving force is small, the effective diffusion is reduced from the Brownian diffusion by a factor that increases exponentially with the potential amplitude. This is not surprising. For small driving force, the particle motion is constrained by the static potential. To move by Brownian diffusion from the minimum energy location in one period to that in the next one, the particle has to jump over a energy barrier of the magnitude of the potential amplitude. It is the energy barriers that reduce the effective diffusion exponentially. When the driving force is large, however, the situation is very different. As we will see later, in the case of large driving force, the effective diffusion is actually larger than the Brownian diffusion.

Regime 2 f is large.

We use Watson's Lemma (the Laplace integral method) [19] to expand $w_0(x)$ as

$$\begin{aligned} w_0(x) &= \int_0^1 \exp\left(\phi(x+s)-\phi(x)\right)\mathrm{e}^{-fs}\,\mathrm{d}s \\ &= \int_0^1 \left[1 + s\,\phi'(x) + s^2\frac{1}{2}\left((\phi'(x))^2 + \phi''(x)\right) + O(s^3)\right]\mathrm{e}^{-fs}\,\mathrm{d}s \\ &= \frac{1}{f}\left[1 + \frac{1}{f}\phi'(x) + \frac{1}{f^2}\left((\phi'(x))^2 + \phi''(x)\right) + O\left(\frac{1}{f^3}\right)\right]. \end{aligned}$$

Integrating with respect to x and using the fact that $\phi(x)$ is periodic, we have

$$\int_0^1 w_0(x)\mathrm{d}x = \frac{1}{f}\left[1 + \frac{1}{f^2}\int_0^1 (\phi'(x))^2\mathrm{d}x + O\left(\frac{1}{f^3}\right)\right].$$

Substituting the expansion of $w_0(x)$ into the expression of $\int_0^1 w_1(x)\mathrm{d}x$, we otain

$$\begin{aligned}\int_0^1 w_1(x)\mathrm{d}x &= \int_0^1 w_0^2(x)\int_0^1 \mathrm{e}^{\phi(x)-\phi(x-s)-fs}\,\mathrm{d}s\,\mathrm{d}x \\ &= \frac{1}{f^3}\int_0^1 \left[1+\frac{1}{f}\phi'(x)+\frac{1}{f^2}\left((\phi'(x))^2+\phi''(x)\right)+O\left(\frac{1}{f^3}\right)\right]^2 \\ &\quad\times\left[1+\frac{1}{f}\phi'(x)+\frac{1}{f^2}\left((\phi'(x))^2-\phi''(x)\right)+O\left(\frac{1}{f^3}\right)\right]\mathrm{d}x \\ &= \frac{1}{f^3}\left[1+\frac{6}{f^2}\int_0^1 (\phi'(x))^2\mathrm{d}x+O\left(\frac{1}{f^3}\right)\right].\end{aligned}$$

The effective drag coefficient and the effective diffusion have the expansions:

$$V_{\mathrm{avg}} = \frac{1-\mathrm{e}^{-f}}{\int_0^1 w_0(x)\mathrm{d}x} = f\left[1-\frac{1}{f^2}\int_0^1 (\phi'(x))^2\mathrm{d}x+O\left(\frac{1}{f^3}\right)\right], \tag{54}$$

$$\zeta_{\mathrm{eff}} = \frac{f\int_0^1 w_0(x)\mathrm{d}x}{1-\mathrm{e}^{-f}} = 1+\frac{1}{f^2}\int_0^1 (\phi'(x))^2\mathrm{d}x+O\left(\frac{1}{f^3}\right), \tag{55}$$

$$D_{\mathrm{eff}} = \frac{\int_0^1 w_1(x)\mathrm{d}x}{\left(\int_0^1 w_0(x)\mathrm{d}x\right)^3} = 1+\frac{3}{f^2}\int_0^1 (\phi'(x))^2\mathrm{d}x+O\left(\frac{1}{f^3}\right). \tag{56}$$

Note that as $f \to \infty$, the effective diffusion decreases to 1, the value of the non-dimensionalized Brownian diffusion. That means, for a moderately large driving force, the effective diffusion is larger than the Brownian diffusion.

In the case of large driving force, the Einstein relation is again valid approximately up to $O(1/f)$ term:

$$\zeta_{\mathrm{eff}}\cdot D_{\mathrm{eff}} = 1+\frac{4}{f^2}\int_0^1 (\phi'(x))^2\mathrm{d}x+O\left(\frac{1}{f^3}\right). \tag{57}$$

Thus, the Einstein relation is approximately valid in both the case of small driving force and the case of large driving force. When the driving force is in between these two extreme cases, (57) indicates that the product of the effective diffusion and the effective drag coefficient is larger than 1.

4 Numerical Results

We implement the integral formulas (44) and (45) numerically using Romberg integration method to compute the effective diffusion coefficient and the effective drag coefficient. We carry out numerical simulations for the case where the static periodic potential is

$$\phi(x) = 5\sin(2\pi x).$$

Figure 2 shows the effective diffusion D_{eff} as a function of the driving force f. As we derived in the asymptotic analysis of the previous section, when the driving force is small, the effective diffusion is reduced exponentially to almost zero by the static periodic potential. When the driving force is very large, the effective diffusion converges from above to 1 (the non-dimensional Brownian diffusion), again confirming the results of the asymptotic analysis. For moderately large driving force, the effective diffusion is significantly above the Brownian diffusion. In Figure 2, the effective diffusion attains a maximum at an intermediate driving force. The location of the maximum of the effective diffusion is approximately the smallest driving force f_c that makes

$$-\phi'(x) + f \geq 0 \quad \text{ for all } \ x,$$

where $-\phi'(x) + f$ is the total active force on the particle (the sum of the constant driving force and the force from the periodic potential). For $\phi(x) = 5\sin(2\pi x)$, we have $f_c = 5 \times 2\pi \approx 31.4$.

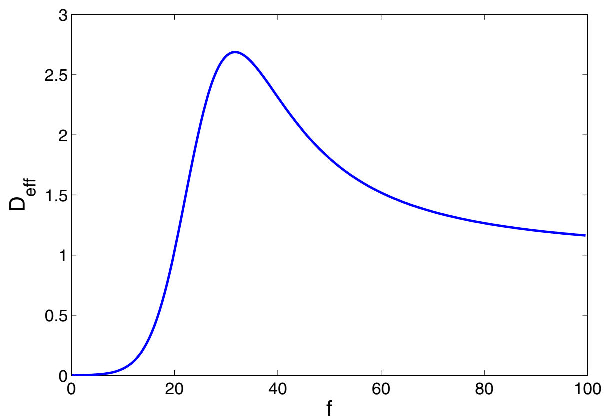

Fig.2 The effective diffusion as a function of the driving force

Figure 3 shows $\zeta_{\text{eff}} \cdot D_{\text{eff}}$, the product of the effective diffusion and the effective drag coefficient, as a function of the driving force f. In the Einstein relation, this product should be 1 (if we use the Brownian drag coefficient and Brownian diffusion). Indeed, in Figure 3, the product $\zeta_{\text{eff}} \cdot D_{\text{eff}}$ does approach 1 for small f and for large f, consistent with the asymptotic results obtained in the previous section. For driving forces in between, the product $\zeta_{\text{eff}} \cdot D_{\text{eff}}$ is always larger than 1, and it attains a maximum at an intermediate force. However, the maximum of $\zeta_{\text{eff}} \cdot D_{\text{eff}}$ is attained at a force appreciably smaller than f_c.

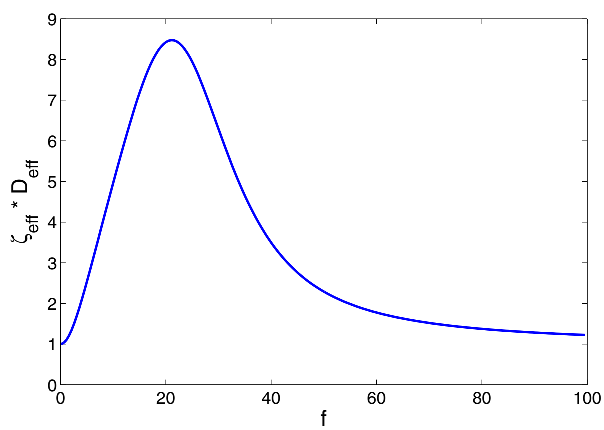

Fig.3 The product of the effective diffusion and the effective drag coefficient as a function of the driving force

5 Discussion

In this paper, we have studied the stochastic motion of a Brownian particle driven by a constant force over a static periodic potential. We have derived integral expressions for the effective diffusion and the effective drag coefficient of the particle. These analytic expressions provide the theoretical foundation for investigating the behavior of the effective diffusion and the effective drag coefficient. With proper implementation, these integral formulas also serve as efficient numerical tools for computing the effective diffusion and the effective drag coefficient. Note that a direct calculation of the effective diffusion involves solving the Fokker-Planck equation [20–22] in a large numerical spatial domain and for a long time, which is computationally expensive and suffers from numerical discretization error. The integral formulas can be evaluated efficiently and with accuracy close to the machine precision by using Romberg integration method.

Based on the analytic expressions, we have studied the asymptotic behaviors of the effective diffusion and the effective drag coefficient, in the regime of small driving force and in the regime of large driving force. It is interesting to compare the asymptotic behaviors in these two cases. As we discussed in the previous sections, for small driving force, the effective diffusion is reduced by a factor that grows exponentially with the amplitude of the potential and the drag coefficient is increased by the same factor. This is primarily caused by that the energy barriers in the static potential decrease the mobility of the particle. In contrast, for large driving force, both the drag coefficient and the effective diffusion are above their Brownian values. It is not very difficult to see why the drag coefficient is above its Brownian value. The static potential barriers slow down the particle motion. In other words, in the absence of the static potential barriers, the particle would move faster. It is, however, not immediately clear how the combination of a static periodic potential and a moderately large driving force increases the effective diffusion. It is important to point that the mechanism of increasing the effective diffusion is definitely a non-linear one. In the absence of a static periodic potential, the effective diffusion is always the same as the Brownian diffusion ($= 1$ after non-dimensionalization). In the absence of a driving force (the limit of small driving force), the static periodic potential decreases the effective diffusion exponentially. Thus, the mechanism of increasing the effective potential must come from the non-linear interaction between the driving force and the static periodic potential. The physical mechanism of the effective diffusion being significantly above the Brownian diffusion will be investigated in a subsequent study.

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