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Suppression of diffusion by a weak external field in periodic potentials

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Abstract. Diffusion of overdamped Brownian particles in sawtooth potentials subject to a spatially uniform tilt is studied focusing on the influence of a small bias. It is shown that in the potentials with an asymmetry in the direction of tilting force, the application of a weak external force leads to a suppression of diffusive motion: the diffusion coefficient as a function of bias passes through a minimum which precedes an increase of diffusion caused by delocalization of particles. In the weak noise limit the effect can be understood as a competition between the forward and backward escape rates over potential barriers determining the behaviour of the diffusion coefficient in a weak external field. The asymptotic lower border for the reduction of spreading of particles at fixed temperature is established. The decrease of diffusion is accompanied by more rapid increase of current.

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Although the transport of Brownian particles in periodic potentials has been a matter of research during a long time [1], several interesting phenomena in this field were discovered only recently [2,4]. First of all, one has to mention the amplification of diffusion caused by an external constant force [2,3] and the non-monotonic dependence of the diffusion coefficient and coherence level of Brownian transport on temperature [3,4]. Similar effects were also established in environments with non-homogeneous dissipation [5] and temperature [6]. In reference [5] a slight decrease of the diffusion coefficient in a symmetric periodic potential with space-dependent friction subjected to a small bias was observed. This unexpected finding indicates that the properties of weakly forced diffusion in periodic structures are not completely understood.

For Brownian motion in a periodic potential loaded by a weak stationary external field, a difference between the forward (in the direction of bias) and backward escape rates from the local minima appears. Such an asymmetry manifests itself in a rise of directed macroscopic transport (current) and has an effect on diffusion. In this letter we show that the influence of a small tilting force on the diffusive motion of the particles depends substantially on the relative behaviour of the escape processes determined by the shape of periodic potential. It proves, in particular, that in the situations where the decrement of backward transitions prevails over the increment of forward transitions, diffusion is suppressed in a weak external field.

Consequently, besides the well-known fact that the diffusion coefficient is always smaller in unbiased periodic potentials compared to the free thermal diffusion [7], there exists a possibility to additionally reduce the spreading of particles by applying a suitable static tilt to the potentials with a certain asymmetry. This effect may be of interest physically as well as for applications, providing an extra factor in controlling the coherence of Brownian transport. In what follows we study this effect in the case of Brownian particles moving in one-dimensional piecewise linear potentials. The results obtained for this simple model may also be useful for understanding of similar phenomena in systems of more complicated spatial structure.

Overdamped motion of a Brownian particle in a tilted periodic potential $V(x) = V_0(x) - Fx$, where $V_0(x)=V_0(x+L)$, and $F \geq 0$ stands for the constant external force, is described by the Langevin equation

$$\eta \frac{dx(t)}{dt} = -\frac{dV(x)}{dx} + \xi(t). \qquad (1)$$

Here η is the viscous friction coefficient and $\xi(t)$ is the zero mean Gaussian white noise with the correlation function $\langle \xi(t)\xi(t')\rangle = 2\eta k_B T \delta(t-t')$. For a simple sawtooth potential with an amplitude A and asymmetry parameter k $(0 \leq k \leq L)$[1] we have $V(x) = A(k-x)/\alpha - Fx$, where $\alpha = k$, if $0 \leq x \leq k$, and $\alpha = k - L$, if $k \leq x \leq L$. If the tilting force exceeds the critical value $F_c = A/(L-k)$,

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[1] The potential is symmetric if $k = L/2$ and, respectively, positively (negatively) asymmetric if $k > L/2$ $(k < L/2)$.

the potential does not have local minima. The diffusion coefficient and current are defined as

$$D = \lim_{t\to\infty} \frac{\langle x^2(t)\rangle - \langle x(t)\rangle^2}{2t}, \qquad v = \lim_{t\to\infty} \frac{\langle x(t)\rangle}{t}. \quad (2)$$

We choose $L = 1$ and replace the relevant quantities with the corresponding dimensionless ones: $\tilde{T} = k_B T A^{-1}$, $\tilde{F} = F/F_c$, $\tilde{F_c} = 1$, $\tilde{D} = D\eta A^{-1}$, and $\tilde{v} = v\eta A^{-1}$. The dimensionless potential is introduced by means of the relation $\tilde{V}/\tilde{T} = V/k_B T$ so that

$$\begin{aligned} \tilde{V}(x) &= a_0 - ax, \quad 0 \le x \le k, \\ \tilde{V}(x) &= -b_0 + bx, \quad k \le x \le 1 \end{aligned} \quad (3)$$

with the notations

$$a_0 = 1, \quad a = \frac{1-(1-\tilde{F})k}{(1-k)k}, \quad b_0 = \frac{k}{1-k}, \quad b = \frac{1-\tilde{F}}{1-k}. \quad (4)$$

Henceforth, the tilde signs above the symbols will be omitted.

On the basis of the general analytical approach developed in references [3] the exact algebraic expressions for the diffusion coefficient and current in the case of tilted piecewise linear periodic potential were derived in reference [8]. In the weak noise limit, if the conditions $(1-F)/T \gg 1$ and $F < 1$ are fulfilled, these expressions simplify substantially (see [8]). In particular, we can present the diffusion coefficient and current for this case in terms of escape rates. An analysis of diffusion in a tilted smooth symmetric potential in the terms of escape statistics was carried out for various damping regimes in reference [9].

In the weak noise limit the transport of particles in a periodic potential subject to a small bias is influenced mainly by the heights of potential barriers. For the piecewise linear potential (3) the right-side and left-side barrier heights read respectively as

$$\begin{aligned} \Delta V_+ &= V(1) - V(k) = 1 - F, \\ \Delta V_- &= V(0) - V(k) = 1 + \frac{k}{1-k}F. \end{aligned} \quad (5)$$

The quantities $\Delta V_\pm$[2] determine the escape rates over the corresponding barriers ($\Delta V_\pm \gg T$)

$$w_\pm = \frac{(\Delta V_+)^2(\Delta V_-)^2}{T} \exp\left(-\frac{\Delta V_\pm}{T}\right). \quad (6)$$

Equations (6) can be obtained using the standard scheme for the derivation of the Kramers formula [10], except the expansion into Taylor series near the extrema of $V(x)$, which is not applicable in the case of a piecewise linear potential. However, in the present case this expansion is not necessary as the relevant integrals can be explicitly calculated. By means of escape rates (6) we can express

[2] Note that the chosen scale of external force depends through the critical tilt on the asymmetry parameter k.

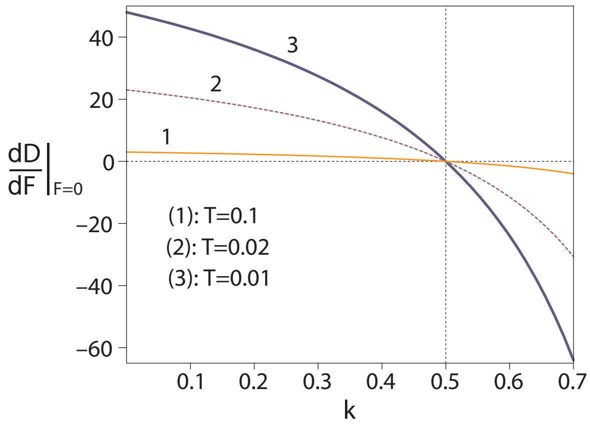

Fig. 1. The plot of the derivative $\partial D/\partial F|_{F=0}$ vs. the asymmetry parameter for various values of temperature.

the diffusion coefficient and current in the following form (see [11]):

$$D = \frac{1}{2}(w_+ + w_-), \quad (7)$$

$$v = w_+ - w_-. \quad (8)$$

Therefore, $D(F)$ and $v(F)$ are completely determined by the rates $w_\pm$ in the relevant approximation. At $F = 0$ we have $D(0) = w$, where $w = T^{-1}e^{-1/T}$ is the escape rate in the untilted potential. Let us reassure that the expressions (7) and (8) are particular cases of the general formula presented in references [3].

Proceeding from equations (7, 8) we analyze the behaviour of diffusion in a weak external field as well the relationship between the properties of diffusion and current in this regime.

The response of diffusion to the application of an infinitesimally weak tilting force is characterized by the slope of the function $D(F)$ in the limit $F \to 0$, that is by the derivative $\partial D/\partial F$ at $F = 0$. The dependence of this quantity on the asymmetry of the periodic potential is shown in Figure 1. As one can see, the slope of $D(F)|_{F=0}$ changes its sign regardless of the temperature if the asymmetry parameter passes the value $k = 0.5$, being positive for $k < 0.5$ and negative for $k > 0.5$. Consequently, if a tiny load is applied, diffusion is reduced in the potentials with positive asymmetry. With the further increase of the tilting force the diffusion coefficient $D(F)$ passes through a minimum (see Figs. 2 and 3) followed by its rise caused by delocalization processes. In the case of the potentials with $k \le 0.5$ the diffusion coefficient increases monotonically if an external field is turned on (see curves 3 and 4 in Fig. 2). The curves depicted in Figures 2 and 3 demonstrate that the suppression of diffusion is favoured by larger values of k and by lower temperatures. The reduction of spreading is maximal in the limit $k \to 1$. Let us also mention that the situation is symmetric with respect to the following transition: $F \to -F$ and $k \to 1-k$.

Equation (7) also enables us to provide a simple interpretation of the discussed suppression of diffusion. The barrier heights $\Delta V_\pm$ vs. F vary at different rates in the

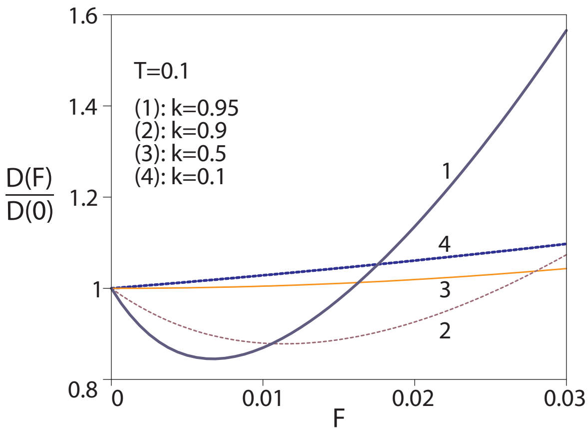

Fig. 2. The plot of the diffusion coefficient vs. the tilting force at fixed temperature for various values of asymmetry parameter.

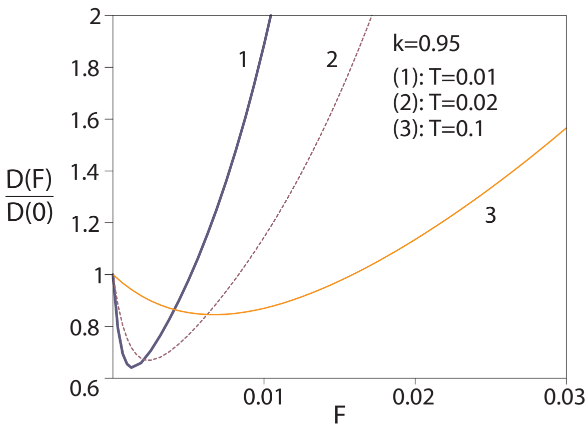

Fig. 3. The plot of the diffusion coefficient vs.the tilting force at fixed asymmetry parameter for various values of temperature.

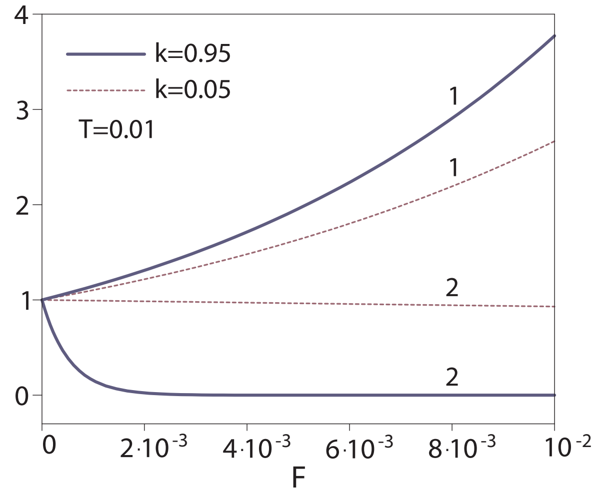

Fig. 4. The plot of the normalized escape rates w_+/w (curves 1) and w_-/w (curves 2) vs. the tilting force at fixed temperature for the periodic potentials of various asymmetry.

potentials where $k \neq 0.5$[3], resulting in the asymmetric behaviour of the escape rates $w_\pm$ in an arbitrary weak external field, as illustrated in Figure 4. By that, as one can observe in Figure 4, for a potential with positive asymmetry the escape rate w_- over the left-side barrier diminishes more rapidly compared with the rise of the escape rate w_+ over the right-side barrier if a very small tilting force is applied, which leads to the suppression of spreading. Further the decrease of w_- slows down while the increase of w_+ picks up speed, i.e. the delocalization processes in the direction of bias become dominating, and the diffusion coefficient passes through a minimum. On the other hand, diffusion is promoted by a weak external field in a potential with negative asymmetry whereas the increasing contribution from w_+ prevails anyway over the decrease of w_- in this case.

[3] It follows from equation (5) that in the potentials with $k > 0.5$ the increment of the left-side barrier height overcomes the decrement of the right-side barrier height as the tilting force increases. The situation is opposite for the potentials with $k < 0.5$.

From equation (7) one can evaluate approximately the tilting force $F_{\rm min}$, which corresponds to the minimum of the diffusion coefficient:

$$F_{\rm min} = T(1-k)\ln \Xi(T,k), \tag{9}$$

where

$$\Xi(T,k) = \frac{k\Phi(T,k)[1-k\Phi(T,k)] - 2T(1-k)[2k\Phi(T,k)-1]}{(1-k)\{\Phi(T,k)[1-k\Phi(T,k)] + 2T[2k\Phi(T,k)-1]\}} \tag{10}$$

with the notation

$$\Phi(T,k) = 1 - T(1-k)\ln\left(\frac{k-2T(2k-1)}{1-k+2T(2k-1)}\right). \tag{11}$$

Substituting $F_{\rm min}$ from equation (9) into equation (7), we obtain for the minimal value of the diffusion coefficient $D_{\rm min} \equiv D(F_{\rm min})$ the following expression:

$$D_{\rm min} = \frac{D(0)}{2\Xi^k(T,k)}[1+\Xi(T,k)] \times [1+Tk\ln\Xi(T,k)]^2[1-T(1-k)\ln\Xi(T,k)]^2. \tag{12}$$

According to equation (12), $D_{\rm min}$ decreases with the increase of the asymmetry parameter k as depicted in Figure 5. In this figure one can also observe that the minimum of the diffusion coefficient is deeper for smaller noise intensities. From equation (12) follows the limit

$$\lim_{k\to 1} D_{\rm min} = \frac{D(0)}{2\Xi_0(T)}[1+\Xi_0(T)][1+T\ln\Xi_0(T)]^2 \tag{13}$$

with

$$\Xi_0(T) = \frac{1-2T}{2T} + \ln\sqrt{\frac{1-2T}{2T}}. \tag{14}$$

Equation (13) provides the asymptotic lower boarder for the maximal suppression of diffusion in a weak external

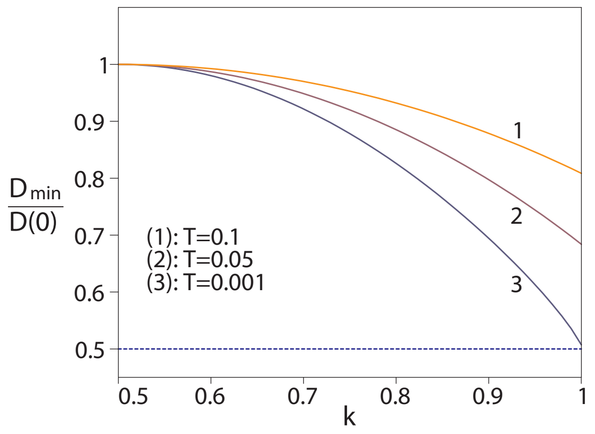

Fig. 5. The plot of the ratio $D_{\rm min}/D(0)$ vs. the asymmetry parameter for various values of temperature.

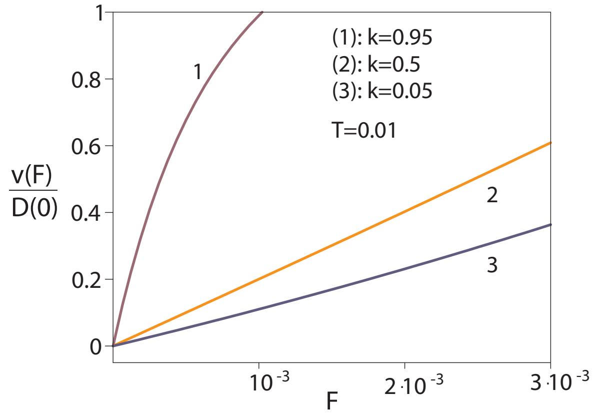

Fig. 6. The plot of the current vs. the tilting force at fixed temperature for various values of asymmetry parameter.

field at fixed temperature. If $T \to 0$, diffusion becomes impossible and the ratio $D_{\rm min}/D(0)$ approaches the lowest value 0.5 when $k \to 1$ (see also Fig. 5). This limiting value associates with the asymptotic behaviour of the escape rates at $F = F_{\rm min}$: if $k \to 1$ and $T \to 0$ then $w_+/w \to 1$ and $w_-/w \to 0$.

Although one can suppress the spreading by means of an external field, the current vs. the tilting force is always increasing due to the different roles of the backward escape processes in the diffusive and directed motion of particles. Furthermore, the acceleration of the current caused by a weak external force is larger just in the potentials where diffusion is reduced by a small bias (see Fig. 6). Such a behaviour becomes comprehensible from the expression of current, equation (8), according to which the rapid fall of the escape rate w_- in a very weak external field applied to a potential with positive asymmetry (see Fig. 4) acts as an additional trigger in the rise of current as bias is turned on. In Figure 6 one should also notice that the current approaches zero with negative curvature if $k > 0.5$ and with positive curvature if $k < 0.5$ consistently with the relation[4] [2]

$$D = T(1-k)\frac{\partial v}{\partial F} \ , \qquad (15)$$

which becomes asymptotically exact in the limit $F \to 0$. Thus, according to equation (15), the dependence of current on tilting force shown in Figure 6 reflects equivalently with Figure 1 the peculiarities of the behaviour of diffusion in the potentials with various asymmetry subject to a weak external field.

The described interrelation between current and diffusion manifests itself in the dependence of the level of coherence of Brownian transport, characterized by the Péclet number $\mathrm{Pe} = v/D$ [3,4,8], on tilting force. In the weak noise limit we obtain on the basis of equations (7) and (8) that $\mathrm{Pe} = 2(w_+ - w_-)/(w_+ + w_-)$. In the external field the Péclet number (the level of coherence) increases and approaches the value $\mathrm{Pe} = 2$ if $w_-/w_+ \ll 1$, which corresponds to the Poissonian hopping process. By that the system reaches the Poissonian regime earlier in the case of positive potential asymmetry due to the suppression of diffusion and the more rapid enhancement of current in the pre-Poissonian region. With the further increase of the tilting force the unidirectional one-step hopping nature of transport is preserved until the inequality $\Delta V_+ \gg T$ holds (see also [8]). However, if the latter condition is violated by a sufficiently strong external field (i.e., the approximate equations (7) and (8) are not applicable anymore), the Péclet number starts to increase, as it was found in reference [8] on the basis of the general scheme of references [3].

The broken spatial inversion symmetry of the periodic system is one of the possible conditions for the appearance of the Brownian motor effect [11–13]. We demonstrated that the special case of this symmetry breaking leads to the decrease of spreading and to the increase of current of particles if a small stationary bias has been applied. Thereby the suitable asymmetry of a periodic potential favours the enhancement of the coherence of Brownian motion in a weak external field. This result may have a certain relationship with the conditions for the suppression of the fluctuations of current and for the increase of rectification efficiency in Brownian motor transport studied recently in reference [14].

In conclusion, in asymmetric periodic potentials one can observe a suppression of diffusion caused by a stationary tilt. A similar effect was reported by Dan and Jayannavar in reference [5] for Brownian particles moving in a symmetric periodic potential with the spatially harmonic friction shifted in phase with respect to the potential. This difference of phases introduces obviously an asymmetry into the resulting force which has spatially varying influence on a particle. Thus it seems that one can speak here more generally about a special spatial anisotropy in the dynamics of Brownian particles required for the reduction of diffusion in a weak external field.

[4] The pre-exponential factor $1-k$ in equation (15) appears in connection with the definition of the dimensionless tilting force used in the present letter.

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