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PECULIARITIES OF BROWNIAN MOTION DEPENDING ON THE STRUCTURE OF THE PERIODIC POTENTIALS*

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Transport of over-damped Brownian particles in periodic double-barrier potentials is studied in the absence and under the influence of a constant tilting force. Depending on the value of the tilt the transport of particles in potentials with two barriers per period has in general character similar to that in simple potentials, exhibiting at the same time in certain parameter regions qualitatively different features. As the most unexpected result it is found that diffusion coefficient can have two maxima. It is also shown that in the wide range of tilting force the transport can be realized through two different Poissonian processes, having at a certain tilt a resonant-like enhancement of the coherence.

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Brownian motion in periodic structures is a relevant problem in several fields of physics, being very interesting from technological, experimental, as well as theoretical point of view, and has been a subject of intense investigations already many years [1–3]. It represents a model that can be applied to numerous systems, ranging from superionic conductors [4] and intercalation compounds to sub-monolayer films adsorbed on surfaces of crystalline substrates [5], weakly pinned charge-density-wave condensates [6], and Josephson junctions [7]. These systems consist of particles that are fixed around certain equilibrium sites and form a regular lattice, and of particles that are mobile and move through this lattice. In Ref. [2] it was shown that the effect of any one-dimensional periodic field is to produce a macroscopic diffusion

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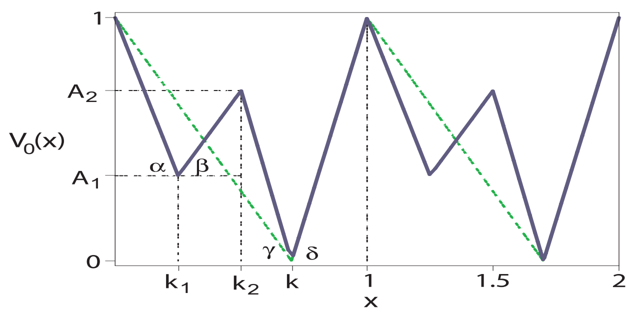

Fig. 1. The general shapes of the periodic potentials. Solid line: piecewise linear double-barrier potential; dashed line: simple sawtooth potential. The potential barrier with the unit-height we call to be the main barrier, and the one with the height $\Delta = A_2 - A_1 < 1$ the additional barrier of the double-barrier potential. The parameters k_1, k_2 and k define the positions of the extrema of the potential, while the quantities α, β, γ and δ represent the slopes (forces).

constant which is always smaller than the Einstein diffusion constant. Later it was proved in Refs. [8, 9] (see also Ref. [10]) that applying a constant external force the diffusion coefficient can be enhanced compared to the free diffusion.

In the studies of Brownian motion in periodic potentials the easiest choice, and also the mostly exploited one, is to use a simple cosine-type potential. However, in many cases this is an oversimplification and we are closer to a real situation using more complicated potentials (see Ref. [11], and also [12]). As said in Ref. [13] *experimental studies performed on different superionic conductor materials show that a number of the ionic compounds are known in which diffusion of ions occurs in double-well potentials.* Also the molecular-dynamics simulations of self-diffusion on metal surfaces [14] and experimental data for superionic conductors [15] provide the evidences that the potential barriers of different heights are important for understanding of transport processes in corresponding systems. To study double-barrier potentials is of relevance also in modeling the kinetics of motor proteins [16,17].

In the present contribution we will thus study the over-damped motion of Brownian particles in the periodic potentials with two barriers per period (see Fig. 1), focusing on the new features appearing compared to the case of the simple potentials. We consider both possibilities: the Brownian motion just in the periodic potential $V_0(x)$, and also under the influence of a constant force. The system is described by the following Langevin equation

$$\eta \frac{dx(t)}{dt} = -\frac{dV_0(x)}{dx} + F + \xi(t)\,, \tag{1}$$

where $F \geq 0$, η is the viscous friction coefficient, $\xi(t)$ is the zero mean Gaussian white noise with correlation function $\langle \xi(t)\, \xi(t') \rangle = 2\, \eta k_{\mathrm{B}} T\, \delta(t-t')$, and T is the temperature. Though we consider only the equilibrium thermal fluctuations, the results are interesting to compare with the ones obtained in Ref. [12] for the over-damped Brownian particles in a potential composed of N hills within one period, driven also by symmetric dichotomic fluctuations.

The basic quantities of our interest are the effective diffusion coefficient and the average particle current defined as:

$$
\begin{aligned}
D &= \lim_{t\to\infty} \frac{\langle x^2(t)\rangle - \langle x(t)\rangle^2}{2t}\,, \\
\langle \dot{x} \rangle &= \lim_{t\to\infty} \frac{\langle x(t)\rangle}{t}\,.
\end{aligned}
\tag{2}
$$

The third quantity, we are interested in, is the Péclet number

$$
\mathrm{Pe} = \frac{L\langle \dot{x} \rangle}{D}\,, \tag{3}
$$

which characterizes the relationship between the directed and diffusive movement of a Brownian particle [9]. Proceeding from the general scheme developed in Ref. [8] we derived exact algebraic expressions for these quantities in the case of the simple sawtooth potential (the calculations and results are revealed in Ref. [18]), and also in the presence of an additional potential trap (see Ref. [20]). In our calculations we took, with no loss of generality, the period $L = 1$ and replaced the relevant quantities with the dimensionless ones: $\tilde{F} = F/F_c$, where $F_c = A/(L-k)$ corresponds to the disappearance of the main potential barrier, and $\tilde{T} = k_{\mathrm{B}} T A^{-1}$, $\tilde{D} = D\eta A^{-1}$, $\tilde{D}_0 = D_0 \eta A^{-1}$ so that $\tilde{D}_0 = \tilde{T}$ and $\langle \tilde{\dot{x}} \rangle = \eta A^{-1} \langle \dot{x} \rangle$. We also chose $A = 1$. For brevity, in what follows, we will omit the tilde signs above the symbols. Thus, all the dependencies, we plot in this paper, are dimensionless and are based on the explicit expressions for the diffusion coefficient, current, and Péclet number.

The analytic result for the diffusion coefficient, presented in Ref. [20], is valid for an arbitrary value of the temperature and the tilting force. Now, if $F = 0$ then $D = Z^{-1}$, where the statistical sum can be divided into two parts, $Z = Z_1 + Z_2$ with

$$
\begin{aligned}
Z_1 \;=\; 2T\biggl\{ & g_{\delta\alpha}\, g_{\alpha\beta} \left[\cosh \frac{1-A_1}{T} - 1\right] + g_{\alpha\beta}\, g_{\beta\gamma} \left[\cosh \frac{A_2 - A_1}{T} - 1\right] \\
& + g_{\beta\gamma}\, g_{\gamma\delta} \left[\cosh \frac{A_2}{T} - 1\right] + g_{\gamma\delta}\, g_{\delta\alpha} \left[\cosh \frac{1}{T} - 1\right] \biggr\}\,,
\end{aligned}
\tag{4}
$$

$$
Z_2 = -2T\left\{ g_{\alpha\beta}\, g_{\gamma\delta} \left[\cosh \frac{A_1}{T} - 1\right] + g_{\delta\alpha}\, g_{\beta\gamma} \left[\cosh \frac{1-A_2}{T} - 1\right] \right\}, \tag{5}
$$

where

$$g_{\mu\nu} = \frac{1}{\tan\mu} + \frac{1}{\tan\nu}\,,$$

with $\mu, \nu = \alpha, \beta, \gamma, \delta$ (see Fig. 1).

The four terms in Z_1 correspond to the four potential barriers that particle overcomes per period due to the diffusive motion, and that are in general of different heights. The higher these barriers are compared to the temperature, the bigger is the factor Z_1 and the more suppressed is the spreading. The coefficients $g_{\mu\nu}\, g_{\nu\sigma}$ take into account the shape of the minimum as well as the shape of the maximum of the potential associated with the corresponding barrier. The two terms in Z_2 take into account the differences of the extrema from the minimum value $A_1 = 0$ and from the maximum value $A_2 = 1$.

For the potentials with $\Delta = A_2 - A_1 = 1$ the factor $Z_2 = 0$. Whereas now $g_{\delta\alpha}\, g_{\alpha\beta} + g_{\alpha\beta}\, g_{\beta\gamma} + g_{\beta\gamma}\, g_{\gamma\delta} + g_{\gamma\delta}\, g_{\delta\alpha} = 1$, then Z_1 does not depend on the values of the asymmetry parameters $k_{1,2}$ and k (see Fig. 1) anymore, and $Z = Z_1 = 2T\left[\cosh(T^{-1}) - 1\right]$ like in the case of the simple sawtooth potential. However, in the following we assume that $\Delta < 1$, and then $Z_2 < 0$.

If we consider now a Brownian particle moving in a bistable potential, that is $A_1 = 0$ but $A_2 \neq 1$, then

$$\begin{aligned} Z_1 &= 2T\, g_{\alpha\beta\gamma\delta} \left\{ g_{\beta\gamma} \left[\cosh\frac{\Delta}{T} - 1 \right] + g_{\delta\alpha} \left[\cosh\frac{1}{T} - 1 \right] \right\}, \\ Z_2 &= -2T\, g_{\beta\gamma}\, g_{\delta\alpha} \left[\cosh\frac{1-\Delta}{T} - 1 \right]. \end{aligned} \tag{6}$$

If instead $A_2 = 1$ and $A_1 \neq 0$ then the potential is metastable and

$$\begin{aligned} Z_1 &= 2T\, g_{\alpha\beta\gamma\delta} \left\{ g_{\alpha\beta} \left[\cosh\frac{\Delta}{T} - 1 \right] + g_{\gamma\delta} \left[\cosh\frac{1}{T} - 1 \right] \right\}, \\ Z_2 &= -2T\, g_{\alpha\beta}\, g_{\gamma\delta} \left[\cosh\frac{1-\Delta}{T} - 1 \right]. \end{aligned} \tag{7}$$

In Eqs. (6) and (7)

$$g_{\alpha\beta\gamma\delta} = \sum_{\mu=\alpha,\beta,\gamma,\delta} \frac{1}{\tan\mu}\,.$$

In the case of a symmetric metastable potential $\alpha = \beta$ and $\gamma = \delta$, for the bistable one $\alpha = \delta$ and $\beta = \gamma$, and one can see that the quantities Z_1 and Z_2, and thus the diffusion coefficient, coincide for the same values of Δ for the two types of potentials. If the potentials are asymmetric then the behavior of the diffusion coefficients D *versus* Δ can be different. The dependence of the

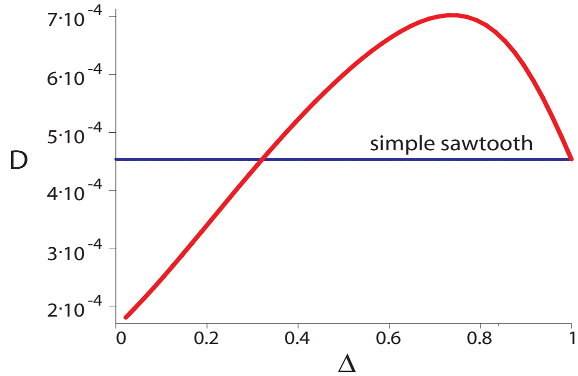

Fig. 2. Diffusion coefficient D as a function of Δ in the symmetric bi- and metastable periodic potentials in the absence of an tilting force; $T = 0.1$.

diffusion coefficient in symmetric bi- and metastable potentials *versus* the additional barrier height is illustrated in Fig. 2. In this figure one can also see that it is possible to have a situation where the diffusion in a potential with two minima per period is suppressed compared to the case of a simple sawtooth potential, though from the condition $Z_2 < 0$ one could assume that an additional trap in general should promote diffusion. However, if the value of Δ is sufficiently small the effective potential contains the segments where the deterministic force is approximately zero, which causes the decrease of diffusion (*cf.* Ref. [20]. Comparable results for the behavior of $D(\Delta)$ are found in Ref. [13] at a high friction regime. However, in Ref. [13] the motion is not still completely over-damped and the diffusion coefficient rises at the values $\Delta \to 0$ which obviously is an effect of the inertia of a particle. In the over-damped limit such a region is absent and the value of diffusion coefficient at $\Delta = 0$ is

$$D = 2\left[T\left(\cosh\frac{1}{T} - 1\right) + \sinh\frac{1}{T} + \frac{1}{2T}\right]^{-1}. \tag{8}$$

Now, if the Brownian particle is in a simple sawtooth potential with a positive asymmetry ($k > 1/2$) and there is a very small constant force influencing the system, then the diffusion is suppressed respect to the spreading at $F = 0$ (see Ref. [21], but also [22]). The same is valid for a double-well potential if at least one of the potential minima is asymmetric to the right, this means $k_1 > k_2/2$ or/and $k > (1 - k_2)/2$. Furthermore, for a certain type of potential shape one can observe the suppression of diffusion also at the larger tilting forces giving rise to a double-maximum in the diffusion coefficient $D(F)$, as demonstrated in Fig. 3. In fact, astonishing is not

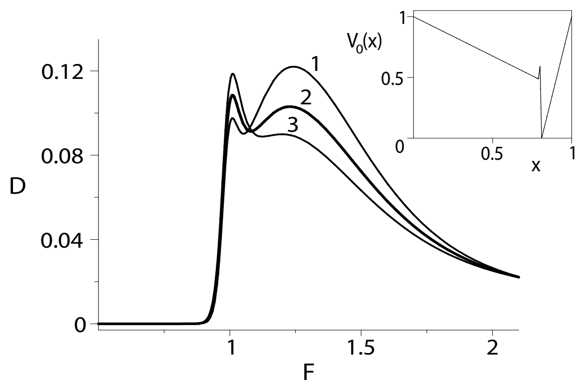

Fig. 3. The existence of two maxima for diffusion coefficient *versus* tilting force: (1): $T = 0.0095$; (2): $T = 0.01$; (3): $T = 0.0105$. The potential parameters are $k_1 = 0.79$, $k_2 = 0.8$, $k = 0.81$, $A_1 = 0.888$, $A_2 = 1$; the corresponding periodic potential is also depicted.

the suppression of the spreading, but the increase of the diffusion coefficient after the decrease. To obtain such a double-enhancement the slope of the additional potential barrier must be much bigger compared to the one of the main barrier, and the height of the barrier must be relatively small ($\Delta = 10T$, $T \approx 1/100$). The decrease of the diffusion coefficient *versus* tilting force takes first of all place due to the disappearance of the main potential barrier. At the tilting force $F = 1$ particle can be in the region of free diffusion or trapped in the additional potential minimum. In that case for every value of F, which is very slightly larger than the previous value, we can consider the situation to be equal to the one of tilting force close to zero, whereas the actual external force is small compared to the critical force at which the potential has no minima anymore. Thus as an additional effect the spreading is decreased similarly to the suppression which takes place at small values of the tilting, as discussed in [21]. Further the diffusion coefficient increases due to the acceleration of diffusion as it takes place also in the simple potentials, and due to the delocalization process as the effective barrier height gets smaller (see Ref. [21]). Whereas the value of the tilting is actually not zero, but is very large, and the height of the potential barrier is small compared to the temperature, then the diffusion decreases to the free diffusion level already before exceeding the critical tilting.

For most of the potentials with $\beta > \delta$, however, the diffusion coefficient $D(F)$ does not have two maxima, but the acceleration of diffusion is characterized by two regions related to the two potential minima (see Fig. 4). In Refs. [18, 19] we showed, in the case of a simple sawtooth potential, that at low temperatures and for subcritical tilt the coherence level stabilizes to the

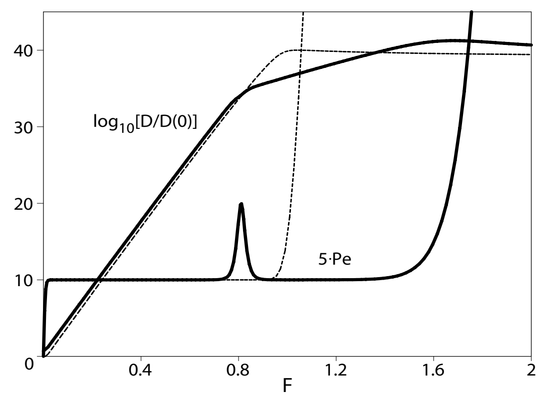

Fig. 4. The comparison of the diffusion coefficient D and Péclet number Pe as the functions of tilting force F. Dashed line: simple sawtooth potential; solid line: double-well potential with $k_1 = 0.3$, $k_2 = 0.38$, $k = 0.65$, $\Delta = 0.4$. Temperature $T = 0.01$.

value $\mathrm{Pe}(F) = 2$. In this parameter region, where the acceleration of diffusion is most essential, the particles are mainly localized around the potential minima and transport is described with great accuracy by the Poissonian hopping process (see Ref. [18]).

Now, for the double-well potentials with $\beta > \delta$ there exists a threshold value of the tilting force

$$F_0 = \frac{(1-\Delta)(1-k)}{1-k-\Delta k}\,, \qquad \Delta k = k_2 - k_1\,, \tag{9}$$

at which the main potential barrier becomes smaller than the additional barrier. If $F < F_0$, particles are mainly localized near the primary traps, whereas if $F > F_0$, near the extra traps. As a result the acceleration of diffusion *versus* tilting force is realized through two different Poissonian processes. As seen in Fig. 4, the two regions of the acceleration of diffusion correspond to these different Poisson processes. Thereby the Poissonian process in the first region coincides with the one which takes place in the corresponding simple sawtooth potential.

In the region of crossover between the two regimes of the enhancement of diffusion, the Péclet number passes through a sharp maximum with the characteristic value $\mathrm{Pe} = 4$. Thus, in a certain region of the tilting force a small variation of the potential has an influence on the character of transport (*cf.* Ref. [23]). The observed enhancement of coherence appears in the region, where the acceleration regime of diffusion and current changes, whereas the increase of diffusion slows down compared to the increase of current. In this case the average populations of the primary traps and the extra traps are close to each other and the possibility of the localization of Brownian particles near the minima of both types is considerable, leading to the relative suppression of diffusion. The suppression is the largest if both of the potential traps are switched on with equal weights. Such a doubling of the effective number of the localization centers in the region of Poissonian process gives a qualitative explanation for the universal value of Péclet number $\mathrm{Pe} = 4$.

In Fig. 5 one can see that for the existence of the extremum in the coherence of Brownian motion *versus* tilting force it must be valid that $\beta > \delta$. If this condition is not fulfilled then the Brownian motion is in the region of subcritical tilting described by one Poissonian process that

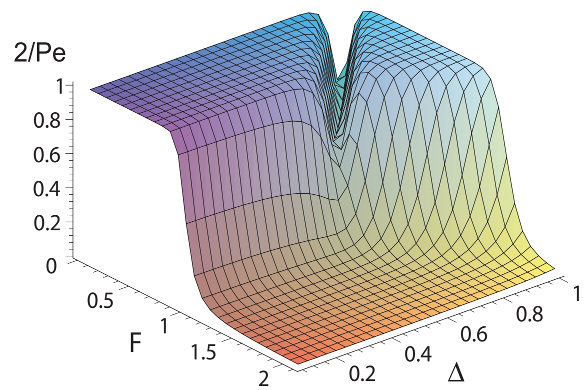

Fig. 5. $2/\mathrm{Pe}$ (randomness parameter) *versus* tilting force F and Δ. Asymmetry coefficients are: $k_1 = 0.35$, $k_2 = 0.5$, $k = 0.75$; if $\Delta = 0.6$ then $\beta = \delta$. Temperature $T = 0.02$.

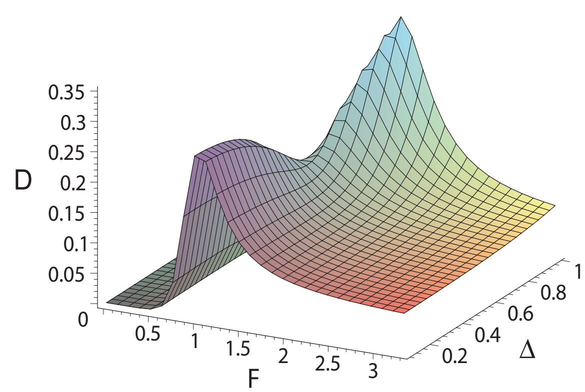

Fig. 6. Diffusion coefficient D as a function of the tilting force F and Δ. The potential parameters are the same as in Fig. 5. Temperature $T = 0.05$.

corresponds to the one in the primary potential traps and there are no special peculiarities one could talk about (*cf.* Ref. [12]), expect that the diffusion coefficient is suppressed compared to the one in the corresponding simple sawtooth potential, in the same reason as discussed for the case $F = 0$ (see also Ref. [20]). As shown in Fig. 6 the suppression of diffusion is most essential at the value Δ so that $\beta = \delta$ for the given asymmetry parameters, due to the doubling of the effective potential traps. For the values of Δ for which $\beta > \delta$ the maximal value of the diffusion coefficient increases and we obtain the discussed enhancement of coherence in the region of subcritical tilting force.

To conclude, we emphasize that the model of a Brownian particle moving in a periodic potential with two barriers per period turns out to be unexpectedly rich and flexible. This provides a possibility to describe in the different regions of the space of the system parameters various effects, which may be of relevance in condensed matter physics and molecular biology.

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