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# Diffusion and coherence of Brownian particles in tilted periodic potentials

Master Thesis in Theoretical Physics

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# Contents

# 1 Introduction

It is difficult to overestimate the importance of the effects caused by Brownian motion for soft condensed matter physics. An object of special attention has been Brownian motion in periodic structures, which has various applications in condensed matter physics, chemical physics, nanotechnology, and molecular biology [1, 2, 3, 4]. Furthermore, the idea that adding noise to deterministic motion can give nontrivial results has led to many important discoveries, such as stochastic resonance [5], resonant activation [6], noise-induced spatial patterns [7], noise-induced multistability as well as noise-induced phase transitions [3, 8, 9, 10, 11], ratchets [2], and hypersensitive transport [12], to name just a few of the new phenomena in this field.

Thermal diffusion of Brownian particles in tilted periodic potentials has been an active field of research in recent years [13, 14, 15, 16]. In Ref. [13] overdamped and underdamped motion was considered and the phenomenon of the enhancement of diffusion was found. Refs. [14, 15] provided an analytic description of the effect. A giant amplification of diffusion up to fourteen orders of magnitude was predicted in Refs. [15] and a nonmonotonic behavior of the diffusion coefficient as a function of temperature was found in Ref. [14]. Whereas Refs. [16, 17] describe analogue effects observed in systems with spatially periodic friction coefficient and temperature, respectively.

Usually, when addressing diffusion enhancement, a tilted harmonic spatial periodic potential is used. However, it is known that some features of the ratchet transport mechanism (e.g., the current reversals [18]) are extremely sensitive to the shape of the potential.

The aim of the present work is to carry out a comprehensive study of the dependence of diffusive and coherent motion of overdamped Brownian particles on temperature and tilting force for various shapes of tilted periodic potentials. The target can be achieved in great accuracy using piecewise linear potential.

Piecewise linear potential is important for at least three reasons: It can be used as a first approximation of the shape of arbitrary potential, and it is sufficiently simple to allow an exact algebraic treatment of the relevant quantities. The third feature is that varying only some parameters it is possible to obtain a new shape of the potential, enabling to use the same analytic equations for the quantities under investigation.

The study consists of two parts. First we investigate the overdamped Brownian motion in tilted simple sawtooth potentials, which provides all the effects characteristic of tilted periodic potentials with one minimum per period. As a surprising result we show that this particular simple model allows one to obtain also all the phenomena attained in systems with spatially periodic temperature [17] and nonhomogenous dissipation [16]. Secondly, we study the transport of Brownian particles in tilted piecewise linear potentials with two potential barriers per period. This particular case is of great importance, whereas in order to describe many systems in biology and condensed matter physics, more complicated potentials than the simple sawtooth type potential are required. The transport properties in potentials of such a type have in general a similar character as in the simple potentials, exhibiting at the same time in certain parameter regions qualitatively different features. Although being often extremely sensitive to the potential and environment parameters, these features can be relevant in some complicated systems, in particular in biology.

The results of this study have been published in Physical Review E and Physica A (see List of publications).

## 2 Basic concepts

The aim of this Section is to give a background of the basic concepts of Brownian motion, which are relevant to the rest of the present work. This will be done in the framework of the Langevin equation, in which the presence of a thermal environment is taken into account through the superposition of a damping and a fluctuating random force.

### 2.1 Langevin equation

If a particle of mass $m$ is immersed in a fluid, a friction force will act on the particle. The simplest expression for such a friction or damping force $F_d$ is given by Stoke's law

$$F_d = -\eta v \,, \tag{2.1}$$

where $v$ is the velocity of the particle and $\eta$ is the coefficient of viscous friction. Stoke's law (2.1) is valid if the particle is so large that there are many simultaneous collisions of the fluid molecules with it and if the velocity is low enough so that there is no turbulence. For a spherical particle the coefficient of viscous friction reads

$$\eta = 6\pi\gamma R \,, \tag{2.2}$$

where $R$ is the radius of the particle and $\gamma$ is the viscosity.

Therefore, according to Newton's law, the equation of motion for the particle in the absence of additional forces has the form

$$m\frac{\mathrm{d}v}{\mathrm{d}t} + \eta\, v = 0 \,. \tag{2.3}$$

Thus an initial velocity $v(0)$ decreases to zero according to the law

$$v(t) = v(0)e^{-t/\tau} \,, \tag{2.4}$$

with a relaxation time $\tau = m/\eta$.

The physical mechanism underlying friction is the collision process between the molecules of the fluid and the particle. The momentum of the particle is transferred to the molecules of the fluid and therefore the velocity of the particle decreases to zero. The differential equation (2.3) is a deterministic equation, i.e., the velocity $v(t)$ at time $t$ is completely determined by the initial value according to (2.4). However, Eq. (2.3) is valid only if the mass of the particle is large so that its velocity induced by thermal fluctuations is negligible.

We now take into account the fact that the environment is a heat bath at thermal equilibrium having temperature $T$. We also assume that all transients have died out and the particle is in thermal equilibrium with the bath. From the equipartition law, it is known that in equilibrium the mean kinetic energy of the particle reaches (in one dimensional dynamics) the value

$$\frac{1}{2}m\langle v^2\rangle = \frac{1}{2}k_B T\,, \tag{2.5}$$

where $k_B$ is Boltzmann's constant. For a small enough mass $m$ the thermal velocity $v_{th} = \sqrt{k_B T/m}$ may be observable and therefore the velocity of the particle can no longer be described exactly by Eq. (2.3) with the solution (2.4): The particle will be in an animated and irregular state of motion.

If the mass of the particle is still large compared to the mass of the molecules, one expects (2.3) to be valid approximately. Therefore, it must be modified so that it leads to the correct thermal energy (2.5). The result is achieved by adding a stochastic force $\xi(t)$ to the right-hand side of Eq. (2.3), i.e., the total force $F(t)$, due to the molecules acting on the Brownian particle, is now decomposed into a continuous damping force $F_d(t)$ and a fluctuating force $\xi(t)$ [19] (cf. also Ref. [20, 21]):

$$F(t) = F_d(t) + \xi(t) = -\eta v(t) + \xi(t)\,. \tag{2.6}$$

The properties of the random force $\xi(t)$, which is also called Langevin's force, are given only on average.

Thus, Brownian motion is the motion of a macroscopically small but microscopically large particle that is subject to the collisional forces exerted by the molecules of a surrounding fluid. Considering Eq. (2.6) the equation of motion of the Brownian particle is given as

$$m\frac{\mathrm{d}v(t)}{\mathrm{d}t} = -\eta v(t) + \xi(t)\,. \tag{2.7}$$

Equation (2.7) is called Langevin's equation and was the first example of stochastic differential equation — a differential equation which contains a stochastic term $\xi(t)$.

The method of the Langevin equation gives a natural way for a stochastic generalization of the deterministic description. However, an adequate mathematical grounding for the approach of Langevin was not available until more than 40 years later, when Itô provided his formulation of stochastic differential equations [22].

## 2.2 Gaussian white noise

The right-hand side of Eq. (2.7) represents the effects of the thermal environment — energy dissipation, modelled as viscous friction, and randomly fluctuating forces in the form of the thermal noise $\xi(t)$. These two effects are not independent of each other since both of them have the same origin, namely the interaction of the particle with a huge number of microscopic degrees of freedom of the environment.

The assumptions of the environment being at thermal equilibrium and of a dissipation mechanism of the form $-\eta v(t)$ completely fix the statistical properties of the fluctuations $\xi(t)$ in Eq. (2.7).

The fact that the friction force on the right hand side of Eq. (2.7) is linear in $v(t)$, i.e., no spatial direction is preferred, suggests that, due to their common origin, also the thermal fluctuations are unbiased, that is

$$\langle \xi(t) \rangle = 0\,, \tag{2.8}$$

for all times $t$, where $\langle \ldots \rangle$ indicates the average over independent realizations of the random process $\xi(t)$. The condition (2.8) ensures also that the equation of motion of the average velocity $\langle v(t) \rangle$ is given by the deterministic limit (2.3). Similarly, the fact that the friction force only depends on the present state of the system and not on what happened in the past has its counterpart in the assumption that the random fluctuations are uncorrelated in time, i.e.,

$$\langle \xi(t)\xi(t') \rangle = 0 \quad \text{if} \quad t \neq t'\,. \tag{2.9}$$

Furthermore, the fact that the friction involves no explicit time dependence has its correspondence in the time-translation invariance of all statistical properties of the fluctuations, i.e., the noise $\xi(t)$ is a stationary random process. Finally, the continuity of the friction force in time indicates that the same is valid for the fluctuations. During a small time interval the effect of the environment thus consists of a large number of small and, according to Eq. (2.9), practically independent contributions. Due to the central limit theorem [23] the net effect of all these contributions on the particle coordinate $x(t)$ will thus be Gaussian distributed.

Bearing in mind all these features one can obtain the fluctuation-dissipation relation [1, 2, 24],

$$\langle \xi(t)\,\xi(t') \rangle = 2\,\eta k_B T\,\delta(t - t')\,, \tag{2.10}$$

where $\delta(t - t')$ is Dirac's $\delta$-function. The quantity $2\eta k_B T$ is called the intensity of the noise or the noise strength of the Langevin force [1]. Since $\xi(t)$ is a Gaussian random process, all its statistical properties are completely determined [1, 23, 25] by the mean value (2.8) and the correlation function (2.10). The only particle property which enters the characteristics of the noise is the friction coefficient $\eta$, which may thus be viewed as the coupling strength to the environment.

A noise force with the $\delta$-correlation (2.10) is called white noise, because the spectral distribution [1], which is given by the Fourier transform of (2.10), is independent of frequency. If the stochastic forces are not $\delta$-correlated, i.e., if the spectral density depends on frequency, one uses the term colored noise. White noise does not exist as a physically realizable process. It is, however, fundamental in a mathematical, and indeed in a physical sense, in that it is an idealization of many processes that do occur. Furthermore, situations in which white noise is not a good approximation can often be indirectly expressed quite simply in terms of white noise [22]. In this sense, white noise is the starting point from which a wide range of stochastic descriptions can be derived.

## 2.3 Einstein's relation

Particles, described by the equation of motion in the form (2.7), exhibit free thermal diffusion, whereas there are no additional external forces acting on them.

Multiplying Eq. (2.7) by the position $x(t)$ and averaging over a large number of different particles, one can write,

$$\frac{m}{2}\,\frac{\mathrm{d}^2\langle x^2\rangle}{\mathrm{d}t^2} - m\langle v^2\rangle = -\frac{\eta}{2}\,\frac{\mathrm{d}\langle x^2\rangle}{\mathrm{d}t} + \langle \xi(t)\, x\rangle\,. \tag{2.11}$$

A crucial implicit assumption [22] in Eq. (2.7) is the independence of the friction force, and hence also of the fluctuation force, from the system $x(t)$, i.e.,

$$\langle \xi(t) x(t')\rangle = 0\,, \tag{2.12}$$

for all times $t \geq t'$. It reflects the assumption that the environment can be represented as a heat bath so that its properties are practically not influenced by the behavior of the particle $x(t)$ [2].

Considering the latter fact and Eq. (2.5) one finds that the general solution of Eq. (2.11) is

$$\frac{\mathrm{d}\langle x^2\rangle}{\mathrm{d}t} = \frac{2k_B T}{\eta} + Ce^{-t/\tau}\,, \tag{2.13}$$

where $C$ is an arbitrary constant. For asymptotically large times $t$ (cf. Ref. [1]) one can neglect the last term in Eq. (2.13) [19, 22] and integrate once more to obtain

$$\langle x^2(t)\rangle = 2t\,\frac{k_B T}{\eta}\,. \tag{2.14}$$

Thus, we have for the free diffusion coefficient the expression [26, 22]

$$D_0 = \frac{k_B T}{\eta}\,, \tag{2.15}$$

known as Einstein's relation. Equation (2.15) implies that fluctuation and dissipation are intimately related, and that one cannot be present without the other. However, dissipation would also occur if the collisions with the molecules were not randomly distributed, but occurred at regular intervals. In that case the motion of the particle would be damped, but would not fluctuate and hence Eq. (2.14) would not be applicable. The reason for the relation between dissipation and fluctuation is that the time between collisions is a random variable [21].

# 3 Brownian motion in periodic potentials

This Section tries to yield an inkling of the content of the ratchet model that leads to the specification of the problem of our interest. A short description of the features of Brownian motion in periodic potentials is presented and the definitions of current and diffusion coefficient — the characteristics of macroscopic transport — are given. The closed analytical expression for the current has been derived by Stratonovich in 1958, but it took more than 40 years to obtain a corresponding compact formula for the diffusion coefficient. The review at the end of this Section presents some relevant landmarks from this period.

## 3.1 Ratchet model

The investigation on Brownian motion in periodic potentials originates from the question, whether it is possible — and how — to gain useful work out of unbiased random fluctuations. In the case of macroscopic fluctuations, the task can be accomplished by various types of mechanical and electrical rectifiers. More subtle is the case of microscopic fluctuations when one wants to convert Brownian motion into useful work. The basic idea can be traced back to a talk given by Smoluchowski in 1912 [27], and was later extended by Feynman [28].

The main ingredient of Smoluchowski and Feynman's *Gedankenexperiment* is an axle with at one end vanes and at the other end a so-called ratchet, reminiscent of a circular saw with asymmetric saw-teeth (see Fig. 1). The whole device is surrounded by a gas at thermal equilibrium. So, if it could turn freely around, it would perform a rotatory Brownian motion due to random impacts of gas molecules on the paddles. Whereas the pawl blocks the turns of the axle in one direction and allows it to turn in the other one, it seems quite convincing that the whole gadget will perform on the average a systematic rotation in one direction, even if a small load in the opposite

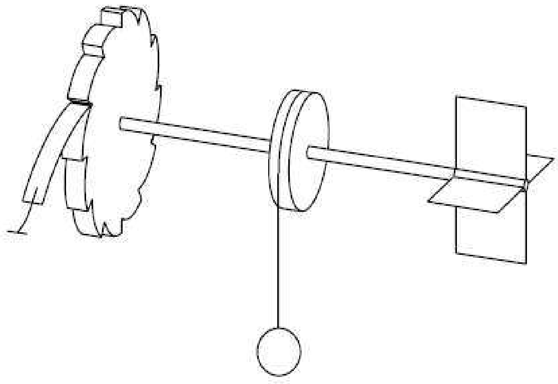

Figure 1: The Smoluchowski-Feynman ratchet and pawl machine.

direction is applied [2]. However, this is in contradiction with the second law of thermodynamics. The paradox of the Smoluchowski-Feynman ratchet is explained in Ref. [28] and a critical analysis of the Feynman gadget is presented in Ref. [29].

In Feynman's lectures [28] one can find an extension of the original *Gedankenexperiment*, where the gas surrounding the two ends of the machine are not at the same temperature — this problem was considered only by Feynman, and is referred to as the Feynman ratchet. The resulting average motion is then nonzero and the efficiency of the device is the same as that of the Carnot cycle. But in this case, a net mean motion of the axle is caused by the macroscopic gradient of temperature.

The Smoluchowski-Feynman ratchet has been experimentally realized on a molecular scale by Kelly, Tellitu, and Sestelo [30]. Their synthesis of triptycene helicene incorporates into a single molecule all essential components: The triptycene "paddle-wheel" functions simultaneously as a circular ratchet and as paddles, the helicene serves as pawl and provides the necessary asymmetry of the system. Both components are connected by a single chemical bond, giving rise to one internal degree of rotational freedom [2]. A discussion of the experimental realizations of the Feynman ratchet can be found in Sec. 4.5 of Ref. [2], and in the references therein.

A faithful modelling and analysis of the ratchet and pawl gadget as it stands is possible but rather involved, especially on a microscopic level (see Ref. [2]). However, one can focus on a considerably simplified mathematical model, which still retains the basic qualitative features, and is formulated as Brownian motion in a one-dimentional spatially periodic potential $V_0(x) = V_0(x+L)$, which corresponds to the ratchet (wheel). Whereas the symmetry of the ratchet is broken, because of the pawl mechanism (teeth are asymmetrical), also the reflection symmetry of the potential is broken: No real number $x'$ exists such that the relation $V_0(x'-x) = V_0(x'+x)$ is fulfilled for every $x$.

Thus, in the case of the Smoluchowski-Feynman ratchet the equation of motion for the particle is

$$m\,\frac{\mathrm{d}^2x(t)}{\mathrm{d}t^2} + \frac{\mathrm{d}V_0(x)}{\mathrm{d}x} = -\eta\,\frac{\mathrm{d}x(t)}{\mathrm{d}t} + \xi(t)\,. \tag{3.1}$$

As we mentioned in Sec. 2.3, the properties of the environment are practically not influenced by the behavior of the system $x(t)$. Especially, the statistical properties of the fluctuations do not depend on the choice of the potential $V_0(x)$, thus Eqs. (2.8) and (2.10) are valid also in the case $V_0(x) \neq 0$.

In Eq. (3.1) the potential force

$$f_0(x) = -\frac{\mathrm{d}V_0(x)}{\mathrm{d}x} \tag{3.2}$$

is zero when averaged over the period $L$:

$$\langle f_0(x)\rangle_L = \frac{1}{L}\int_0^L f_0(x)\,\mathrm{d}x = -\frac{1}{L}\,[V_0(L) - V_0(0)] = 0\,. \tag{3.3}$$

Considering the Feynman ratchet, the equation of motion can be written in the form

$$m\,\frac{\mathrm{d}^2x(t)}{\mathrm{d}t^2} = f_0(x) - \eta\,\frac{\mathrm{d}x(t)}{\mathrm{d}t} + \xi(t) + \zeta(t)\,, \tag{3.4}$$

where one has assumed that instead of the temperature gradient there is a driving nonthermal and nonequilibrium force $\zeta(t)$ of zero mean acting on the system [31].

## 3.2 Overdamped ratchet

### 3.2.1 Equation of overdamped motion

The dynamics of fluctuations of microscopic systems can very often be described within a good approximation with the overdamped dynamics [32, 33]. As an example, we consider the kinesin which is one of the biological (molecular) motors [34]. The kinesin moves along microtubules inside the cells [35, 36, 37] and after its head detaches from the microtubule binding site, it engages in Brownian movement [38]. Microtubules are spatially periodic structures built of tubulin heterodimers which are arranged in rows called protofilaments which, in turn, are oriented nearly parallel to the microtubule axis. A heterodimer is about 8 nm long and is composed of two different globular subunits: $\alpha$- and $\beta$-tubulin. This leads to the reflection symmetry breaking of the microtubules. As a consequence, the corresponding potential $V_0(x)$ with period $L = 8$ nm is asymmetric.

One should note that the velocity $\dot{x} = \mathrm{d}x/\mathrm{d}t$ in Eq. (3.4) is the velocity of the kinesin head during the diffusion phase, which should be distinguished from the overall velocity of the kinesin moving along microtubules. The radius of the kinesin head (the ellipsoidal catalytic core head is approximated as a sphere) is $R = 2.94\,\mathrm{nm}$, and the mass of the head is approximately $m = 6 \times 10^{-20}$ g. The aqueous medium of the cell around the kinesin head has a viscosity of approximately $\gamma = 0.01\,\mathrm{g/cm\ s}$.

Therefore, $\eta = 5.54 \times 10^{-8}$ g/s and the Langevin relaxation time is

$$\tau = 1.08 \times 10^{-12} \text{ s}, \tag{3.5}$$

which is so fast that the inertial term in the equation of motion can be neglected [38]. Hence the second order differential equation (3.4) can be approximated by the first-order differential equation

$$\eta \frac{\mathrm{d}x(t)}{\mathrm{d}t} = f_0(x) + \xi(t) + \zeta(t), \tag{3.6}$$

which describes the overdamped dynamics of Brownian particles. For the above-mentioned example of kinesin it is a very good approximation to the starting model (3.4). We also remark that setting formally $m = 0$ affects neither the fluctuation-dissipation relation (2.10) nor the Einstein relation (2.15).

### 3.2.2 Overdamped ratchet in equilibrium

Under equilibrium conditions, nonthermal fluctuations are excluded, i.e., $\zeta(t) = 0$, and Eq. (3.6) reduces to the form

$$\eta \frac{\mathrm{d}x(t)}{\mathrm{d}t} = f_0(x) + \xi(t), \tag{3.7}$$

which is the "minimal" Smoluchowski-Feynman ratchet model.

Due to the random force $\xi(t)$ it is natural to introduce a statistical ensemble of the stochastic processes in (3.7), related to independent realizations of the random fluctuations $\xi(t)$ [1]. The corresponding probability density $P(x,t)$ at position $x$ and time $t$ describes the distribution of the Brownian particles and follows as an ensemble average of the form

$$P(x,t) = \langle \delta(x - x(t)) \rangle . \tag{3.8}$$

An immediate consequence of this equation is the normalization

$$\int_{-\infty}^{\infty} \mathrm{d}x \, P(x,t) = 1 \,. \tag{3.9}$$

Another straightforward consequence is that $P(x,t) \geq 0$ for all $x$ and $t$.

In order to determine the time-evolution of $P(x,t)$, one can first consider in Eq. (3.7) the special case $f_0(x) = 0$. This corresponds to free diffusion with diffusion constant $D_0$. Consequently, $P(x,t)$ is governed by the diffusion equation

$$\frac{\partial}{\partial t} P(x,t) = D_0 \frac{\partial^2}{\partial x^2} P(x,t) \,. \tag{3.10}$$

Next one can address the deterministic dynamics, obtained by setting $\xi(t) = 0$ in Eq. (3.7). In complete analogy to classical Hamiltonian mechanics, one then finds that the probability density $P(x,t)$ evolves according to a Liouville equation of the form [2]

$$\frac{\partial}{\partial t} P(x,t) = -\frac{\partial}{\partial x} \left[ \frac{f_0(x)}{\eta} P(x,t) \right] \,. \tag{3.11}$$

Since both Eq. (3.10) and (3.11) are linear in $P(x,t)$, the general case follows by combination of both contributions, i.e., one obtains the Kramers equation [1, 25],

$$\frac{\partial}{\partial t} P(x,t) = -\frac{\partial}{\partial x} \left[ \frac{f_0(x)}{\eta} P(x,t) \right] + D_0 \frac{\partial^2}{\partial x^2} P(x,t) \,. \tag{3.12}$$

The first term on the right hand side is the drift term and the second one the diffusion term.

One can also write Eq. (3.12) in the form of a continuity equation for the probability density $P(x,t)$:

$$\frac{\partial}{\partial t} P(x,t) = -\frac{\partial}{\partial x} J(x,t) \,, \tag{3.13}$$

where $J(x,t)$ is the probability current,

$$J(x,t) = \frac{f_0(x)}{\eta}\, P(x,t) - D_0\, \frac{\partial}{\partial x}\, P(x,t)\,. \tag{3.14}$$

Equations (3.13) and (3.14) are valid also for the reduced probability density and current [2] determined as

$$\hat{P}(x,t) = \sum_{n=-\infty}^{\infty} P(x+nL,t)\,, \tag{3.15}$$

$$\hat{J}(x,t) = \sum_{n=-\infty}^{\infty} J(x+nL,t)\,. \tag{3.16}$$

We henceforth devote ourselves to these quantities, taking into account that

$$\hat{P}(x+L,t) = \hat{P}(x,t)\,, \tag{3.17}$$

$$\int\limits_0^L \mathrm{d}x\, \hat{P}(x,t) = 1\,. \tag{3.18}$$

In the stationary state, the density $\hat{P}_{st}(x) = \lim_{t\to\infty} \hat{P}(x,t)$ and the probability current $\hat{J}_{st} = \lim_{t\to\infty} \hat{J}(x,t) = \text{const}$, whereby

$$\hat{J}_{st} = \frac{f_0(x)}{\eta}\, \hat{P}_{st}(x) - D_0\, \frac{\mathrm{d}}{\mathrm{d}x}\, \hat{P}_{st}(x)\,. \tag{3.19}$$

The solution of the Kramers equation for $\hat{P}_{st}(x)$ is

$$\hat{P}_{st}(x) = N^{-1} e^{-V(x)/k_BT}\,, \tag{3.20}$$

$$N = \int\limits_0^L \mathrm{d}x\, e^{-V(x)/k_BT}\,. \tag{3.21}$$

From Eq. (3.7) one obtains, taking (2.8) into account, that

$$\langle \dot{x} \rangle = \frac{\langle f_0(x) \rangle}{\eta} = \int\limits_0^L \mathrm{d}x\, \frac{f_0(x)}{\eta}\, \hat{P}_{st}(x)\,. \tag{3.22}$$

On the basis of Eqs. (3.19) and (3.17), we thus get

$$\langle \dot{x} \rangle = L\hat{J}_{st}\,. \tag{3.23}$$

Whereas for the periodic potential $V_0(x)$, under consideration, $V_0(x+L)-V_0(x)=0$, the average slope of the potential is zero, and the transition rates from a state of local minimum of the potential to the left valley ($\hat{J}_-$) and to the right valley ($\hat{J}_+$) are the same. The stationary mean velocity depends on the difference between the transition rates in the positive and negative directions: $\hat{J}=\hat{J}_+-\hat{J}_-$. Hence, $\hat{J}=0$ and there is no macroscopic transport; This is nothing but detailed balance. In turn, if $\langle \dot{x} \rangle \neq 0$ then the particles perform macroscopic directed motion and stochastic transport occurs in the system.

## 3.3 Tilted Smoluchowski-Feynman ratchet

A chance to violate the principle of detailed balance is to change the constant diffusion coefficient $D_0$ into a diffusion function $D_0(x)$. Diffusive motion with a diffusion coefficient which depends on the state of the system plays an important role in a number of physical systems, e.g., non-linear self-excited oscillators in the presence of noise [39], diodes [25, 40, 41], current instabilities in bulk semiconductors [42] and in ballast resistors [43]; as well as in biological systems [44].

Transport as a consequence of state-dependent diffusion was studied by Büttiker [45] and van Kampen [46]. In Ref. [45] it was demonstrated that the state-dependent diffusion can induce transport in a system which is at equilibrium in the presence of thermal noise only. It was also shown that for small modulation amplitudes the motion of a particle in a periodic potential $V_0(x)$, subject to state-dependent noise, is equivalent to that of a particle subject to thermal noise in the potential

$$V(x)=V_0(x)-Fx\,, \tag{3.24}$$

which consists of a driving force potential $-Fx$ superimposed on the periodic potential $V_0(x)$. The equation of motion can be written in this case as

$$\eta \frac{\mathrm{d}x(t)}{\mathrm{d}t} = f_0(x) + F + \xi(t)\,. \tag{3.25}$$

The last equation is a generalization of the overdamped Smoluchowski-Feynman ratchet model (3.7) in the presence of an additional homogeneous, static force $F$. In the original ratchet and pawl gadget (see Fig. 1) such a force $F$ models the effect of a constant external torque due to a load. This scenario represents a kind of "hydrogen atom" among ratchet models, in that it is one of the few exactly solvable cases.

The solution for the Kramers equation (3.12), where $f_0$ is replaced with $f_0 + F$, is

$$\hat{P}_{st}(x) = \frac{1}{N}\, e^{-V(x)/k_BT} \int\limits_{x}^{x+L} \mathrm{d}y\, e^{V(y)/k_BT}\,, \tag{3.26}$$

$$N = \int\limits_{0}^{L} \mathrm{d}x\, e^{-V(x)/k_BT} \int\limits_{x}^{x+L} \mathrm{d}y\, e^{V(y)/k_BT}\,. \tag{3.27}$$

## 3.4 Transport in periodic potentials

In Secs. 3.1 and 3.2 the periodic potential $V_0(x)$ was assumed to be asymmetrical. However, in the following we do not make such a restriction.

The total potential $V(x) = V_0(x) - Fx$ is a corrugated plane with an average slope determined by the external force $F$, called also tilt (see Fig. 2). The Langevin equation (3.25) describes Brownian motion along such a corrugated plane. There exists a value of the tilting force $F = F_c$ such that for values $F > F_c$ the effective potential $V(x)$ has no minima, whereas for $F < F_c$ minima do occur.

In the systems under the influence of the deterministic and stochastic forces, directed transport and diffusion occur. The quantity of foremost interest in the context of

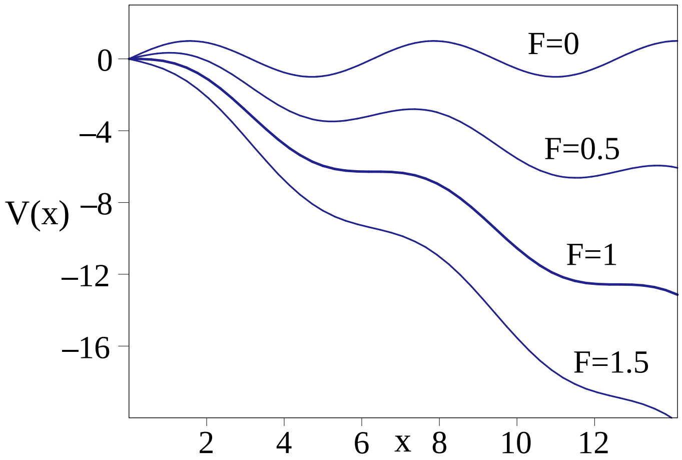


Figure 2: The total potential $V(x) = V_0(x) - Fx$ as a function of $x$ for different values of tilting force $F$; $V_0(x) = \sin(x)$.

transport in periodic systems is the average particle current in the long-time limit, defined as

$$\langle \dot{x} \rangle = \lim_{t\to\infty} \frac{\langle x(t) \rangle}{t} \,, \tag{3.28}$$

while the diffusion coefficient, characterizing the spreading, is

$$D = \lim_{t\to\infty} \frac{\langle x^2(t) \rangle - \langle x(t) \rangle^2}{2t} \,. \tag{3.29}$$

The asymptotic Brownian motion in a tilted periodic potential (3.24) is qualitatively well known. Brownian particles in a tilted washboard subject to friction and noise will diffuse and drift in the direction of the bias.

For a finite value of the tilting force and in the absence of the noise $\xi(t)$ the particle performs, in the overdamped regime, a creeping motion. If minima of the total potential $V(x)$ exist, the particles finally reach them. This solution is called locked solution. If minima do not exist, the particles move down the corrugated plane; This solution is termed running solution. In the presence of noise, the particles do not stay permanently in the locked state but will sometimes be kicked out of their wells, moving to the lower neighboring well and so forth. The particles thus perform a hopping process from one well to the next lower one [1].

In the systems where inertial effects become important, in the absence of the noise a locked solution may occur if minima exist. There may, however, also be a running solution, even if the minima of the potential are present. Because of their momentum the particles may overcome the next hill if the friction constant is small enough. In the presence of the noise, the particles may be kicked out of their well, i.e., out of their locked state. If the damping is small enough, they do not lose their energy very rapidly and therefore they may no longer be trapped in the neighboring lower well, as they are for large friction. The particles may thus get in the running state and may stay in this state for some time. Due to the Langevin forces, the energy of the particle fluctuates; The energy of the particles may thus decrease and they may again be trapped in one of the wells, now again being in the locked state [1]. Low damping diffusion accounts for most inertial effects that play a crucial role in real experiments, e.g. dislocation losses in metals [47], $I - V$ characteristics of shunted Josephson junctions [48, 49], dissipation in certain hysteretic systems [50].

Despite the knowledge of the qualitative behavior of Brownian motion in tilted periodic potential, the determination of the effective diffusion coefficient of the system for arbitrary temperature, bias and periodic potential remained even in the overdamped limit a challenging task for decades, and can be performed in the general damped case only by simulations or by a numerical solution of the Fokker-Planck equation.

The analytical solution for the current (3.28) in tilted periodic potentials goes back to Stratonovich [51] and has subsequently been rederived many times [1, 15, 14].

Stratonovich gave also an approximate expression for the effective diffusion coefficient. This approach holds true for a weak tilting of the potential and small noise intensity. In this case the particle rarely jumps from one potential minimum into the next one to the right or left, whereby one of the directions is preferred due to the bias. Stratonovich assumed that in this regime the process can be modelled by a biased random walk. Thus, the diffusion coefficient is determined by the transition rate from the minimum to the left and right potential barriers (maxima of the potential). This approach neglects the relaxation time from barrier to minimum that becomes relevant for stronger tilt. It fails completely for a so-called supercritical tilt for which minima and maxima of the potential vanish since in this case the process cannot be described by a Poissonian hopping process anymore.

A closed expression for the diffusion coefficient (3.29) in the absence of a tilt $F$ was derived by Lifson and Jackson in Ref. [52] (see also Ref. [53]). They showed that the effect of any one-dimensional non-tilted periodic field is to produce a macroscopic diffusion constant which is always smaller than the free diffusion constant:

$$D = \frac{D_0}{\int_0^L \frac{\mathrm{d}x}{L}\, e^{V_0(x)/k_B T} \int_0^L \frac{\mathrm{d}y}{L}\, e^{-V_0(y)/k_B T}}, \tag{3.30}$$

where the denominator is always larger than unity, by the Cauchy-Schwartz inequality [54].

During the 1970's, an exact expression for the diffusion coefficient was calculated for the special limit of vanishing bias [53, 55] (see also Ref. [1]). Another approximation for a finite bias was used later on by Costantini and Marchesoni in Ref. [13]. They obtained in the overdamped regime an analytic expression which relates the particle diffusion constant to its mobility, and allows one to have an inkling of the enhancement of the diffusion due to the tilting. An unusually large diffusion coefficient was revealed as well in the underdamped regime through numerical simulations.

In 2001, a closed analytical expression for the diffusion coefficient was derived by Lindner *et al.* by mapping the continuous dynamics onto a discrete cumulative process [14], and a nonmonotonic behavior of the diffusion coefficient and coherence level of the transport of Brownian particles as a function of temperature was found. An independent work by Reimann *et al.* [15] led to a similar result, enabling one to obtain a giant acceleration of free diffusion by using tilted periodic potentials in the overdamped regime.

The starting point [15] are the following exact expressions for the particle current and for the diffusion coefficient [15, 56, 57, 58]:

$$\langle \dot{x} \rangle = \frac{L}{\langle t(x_0 \to x_0 + L) \rangle} , \tag{3.31}$$

$$D = \frac{L^2}{2} \frac{\langle t^2(x_0 \to x_0 + L) \rangle - \langle t(x_0 \to x_0 + L) \rangle^2}{\langle t(x_0 \to x_0 + L) \rangle^3} , \tag{3.32}$$

where $x_0$ is an arbitrary reference point and $\langle t^n(a \to b) \rangle$ is the $n$th moment of the first passage time from $a$ to $b > a$ for a stochastic trajectory obeying (3.25), with the assumption that $F > 0$ in order to keep those moments finite. The moments of the first passage time, for the dynamics (3.25), are given by the analytical recursion relation [59]

$$\langle t^n(a \to b) \rangle = \frac{n}{D_0} \int_a^b \mathrm{d}x \, e^{V(x)/k_B T} \int_{-\infty}^{x} \mathrm{d}y \, \langle t^{n-1}(y \to b) \rangle \, e^{-V(y)/k_B T} , \tag{3.33}$$

for $n = 1, 2, \ldots$ and with $\langle t^0(y \to b) \rangle = 1$. By introducing (3.33) into (3.31) and (3.32), one finds the result of Ref. [15], which we will reveal in the next section.

As a further generalization, the approach developed by Reimann *et al.* [15] has been applied in Ref. [16] to show that a non-homogeneous dissipation can induce a minimum in the diffusion coefficient *vs* the applied external force, an enhancement and suppression of the diffusion as a function of temperature, as well as an increase of the order level of the Brownian motion in a tilted symmetric periodic potential (cf. Ref. [60]). Similar anomalies were observed in systems with spatially modulated Gaussian white noise [17] (see also Ref. [14]).

# 4 Brownian motion in tilted piecewise linear periodic potentials: Results

In this Section the results of the thesis are presented. We investigate the overdamped motion of Brownian particles modelled with equation (3.25) in tilted piecewise linear potentials with one and two minima per period. We derive the explicit algebraic expressions for the diffusion coefficient, particle current, and coherence level of Brownian transport. Their dependencies on temperature, tilting force, and the shape of the potentials will be analyzed.

## 4.1 Quantities of interest

Investigating the stochastic transport, the basic quantities of interest are the average particle current in the long-time limit (3.28) and the effective diffusion coefficient on the same time-scale (3.29). The effective diffusion coefficient (3.29) for the model (3.25) with $F \geq 0$ can be written as [15]

$$D = \frac{D_0}{N^3} \int\limits_{x_0}^{x_0+L} \frac{\mathrm{d}x}{L}\, I_+(x)\, I_-^2(x)\,, \tag{4.1}$$

where $x_0$ is an arbitrary point and

$$N = \int\limits_{x_0}^{x_0+L} \frac{\mathrm{d}x}{L}\, I_-(x)\,, \tag{4.2}$$

$$I_\pm(x) = \frac{1}{D_0}\, e^{-FL(1\pm1)/2k_BT}\, e^{\pm V(x)/k_BT} \int\limits_{x}^{x+L} \mathrm{d}y\, e^{\mp V(y)/k_BT}\,. \tag{4.3}$$

The Stratonovich formula [51] for the current can be expressed in the form

$$\langle \dot{x} \rangle = N^{-1}\,(1 - e^{-LF/k_BT})\,. \tag{4.4}$$

The third quantity of interest is the Péclet number, which characterizes the coherence level of Brownian motion [14, 61],

$$\mathrm{Pe} = \frac{L\langle \dot{x} \rangle}{D} \,. \tag{4.5}$$

By coherent motion one means large particle current with minimal diffusion; hence the greater is the Péclet number, the greater the coherence of Brownian transport.

Sometimes it is more convenient to use, instead of the Péclet number, the randomness parameter [62, 63], which is actually measured in experiments, defined as the long time limit of the ratio between the variance of the particle's position and the product of its average position and periodicity,

$$r = \lim_{t\to\infty} \frac{\langle x^2(t) \rangle - \langle x(t) \rangle^2}{\langle x(t) \rangle \, L} \,. \tag{4.6}$$

The definition of the diffusion coefficient and current imply

$$r = \frac{2\, D}{\langle \dot{x} \rangle \, L} \,. \tag{4.7}$$

Thus $\mathrm{Pe} = 2\, r^{-1}$, and it is easy to switch between Péclet number and randomness parameter.

## 4.2 Choice of the potentials and dimensionless units

The piecewise linear periodic potentials with one minimum per period is characterized by the asymmetry parameter $k$: $0 < k < L$. The potential is symmetric if $k = L/2$ (see Fig. 3). The critical tilting force is given by $F_c = A/(L-k)$ , where $A$ is the amplitude of the potential. At the critical tilting $F = F_c$, the force acting on the particle in the region $[k, L]$ is zero.

For the double-periodic potentials we assume that $0 < k_1 < k_2 < k < L$, where $k_1$ corresponds to the additional minimum and $k_2$ to the additional maximum. The

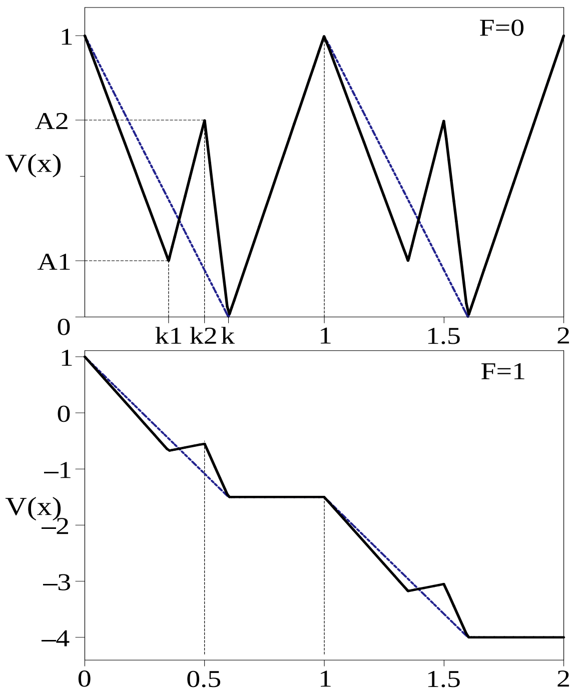


Figure 3: The general shapes of the effective potentials for tilting forces $F = 0$ (above) and for the critical tilt $F = 1$ (below). Solid line: piecewise linear double-periodic potential for $k_1 = 0.35$, $k_2 = 0.5$, $k = 0.6$, $A_1 = 0.2$, $A_2 = 0.7$. Dashed line: simple sawtooth potential for asymmetry parameter $k = 0.6$.

potentials with one and two maxima per period are considered to be comparable for the same values of the parameter $k$, and the corresponding right-hand potential barrier we thus name the primary barrier. In the case of the double-periodic potentials we also assume that $0 \leq A_1 < A_2 \leq A$ and $\Delta A = A_2 - A_1 < A$, whereas we are interested in having an additional trap with a smaller potential barrier than the primary barrier (see Fig. 3). The tilting force corresponding to the disappearance of the additional minima is: $F_{ce} = \Delta A/\Delta k$ , where $\Delta k = k_2 - k_1$.

For the sake of serenity we recast the problem into a dimensionless form [1]. With

[1] Note that all the quantities plotted in the figures are dimensionless.

no loss of generality we take the period $L = 1$ and replace the relevant quantities with the corresponding dimensionless ones: $\tilde{T} = k_B T A^{-1}$, $\tilde{F} = F/F_c$, $\tilde{D} = D\eta A^{-1}$, $\tilde{D}_0 = D_0 \eta A^{-1}$ so that $\tilde{D}_0 = \tilde{T}$ and $\langle \dot{\tilde{x}} \rangle = \eta A^{-1} \langle \dot{x} \rangle$. We also choose $A = 1$ and for brevity, in what follows we will omit the tilde signs above the symbols. Hence,

$$F_{ce} = \frac{\Delta A\,(1-k)}{\Delta k}\,, \qquad F_c = 1\,. \tag{4.8}$$

Considering the case of double-periodic potential, we refer to the critical tilt, as the value $\max(F_{ce}, F_c)$.

The dimensionless potentials, depicted in Fig. 3, are defined as follows ($n = 1, 2, \ldots$ is the number of the period):

(I) Simple sawtooth potential:

$$\begin{aligned} V_{an}(x) &= a_{0n} - ax\,, \qquad (n-1) \le x \le k + (n-1)\,, \\ V_{bn}(x) &= -b_{0n} + bx\,, \qquad k + (n-1) \le x \le n\,, \end{aligned} \tag{4.9}$$

where

$$\begin{aligned} a_{0n} &= 1 + \frac{(n-1)}{k}\,, \qquad a = \frac{1-(1-F)k}{(1-k)k}\,, \\ b_{0n} &= -1 + \frac{n}{1-k}\,, \qquad b = \frac{1-F}{1-k}\,. \end{aligned} \tag{4.10}$$

(II) Double-periodic potential:

$$\begin{aligned} V_{an}(x) &= a_{0n} - ax\,, \qquad (n-1) \le x \le k_1 + (n-1)\,, \\ V_{bn}(x) &= -b_{0n} + bx\,, \qquad k_1 + (n-1) \le x \le k_2 + (n-1)\,, \\ V_{cn}(x) &= c_{0n} - cx\,, \qquad k_2 + (n-1) \le x \le k + (n-1)\,, \\ V_{dn}(x) &= -d_{0n} + dx\,, \qquad k + (n-1) \le x \le n\,, \end{aligned} \tag{4.11}$$

where

$$
\begin{aligned}
a_{0n} &= A_1 + \frac{1-A_1}{k_1}\left[k_1 + (n-1)\right], \qquad a = \frac{1-A_1}{k_1} + \frac{F}{1-k}\,, \\
b_{0n} &= -A_1 + \frac{\Delta A}{\Delta k}\left[k_1 + (n-1)\right], \qquad b = \frac{\Delta A}{\Delta k} - \frac{F}{1-k}\,, \\
c_{0n} &= \frac{A_2}{k-k_2}\left[k + (n-1)\right], \qquad c = \frac{A_2}{k-k_2} + \frac{F}{1-k}\,, \\
d_{0n} &= \frac{1}{1-k}\left[k + (n-1)\right], \qquad d = \frac{1-F}{1-k}\,.
\end{aligned}
\tag{4.12}
$$

## 4.3 Diffusion and coherence in tilted sawtooth potentials with one minimum per period

### 4.3.1 Analytic computations

In the dimensionless units the expressions for the diffusion coefficient, current, and Péclet factor have the following form:

$$D = TYZ^{-3}\,, \tag{4.13}$$

$$\langle \dot{x} \rangle = \varphi_0 Z^{-1}\,, \tag{4.14}$$

$$\mathrm{Pe} = \varphi_0 Z^2 (TY)^{-1}\,, \tag{4.15}$$

where

$$\varphi_0 = 1 - \exp\left(-\frac{F}{T(1-k)}\right)\,, \tag{4.16}$$

$$Z = \int\limits_0^k \mathrm{d}x\, H_{-a}(x) + \int\limits_k^1 \mathrm{d}x\, H_{-b}(x)\,, \tag{4.17}$$

$$Y = \int\limits_0^k \mathrm{d}x\, H_{+a}(x)\, H_{-a}^2(x) + \int\limits_k^1 \mathrm{d}x\, H_{+b}(x)\, H_{-b}^2(x)\,. \tag{4.18}$$

Equations (4.17) and (4.18) contain the functions $H_{\pm a}$ and $H_{\pm b}$ where the subscripts $a$ and $b$ associate, correspondingly, with the limits of integration from 0 to $k$ and from $k$ to 1. Having defined for brevity the generalized potential $v(x) = V(x)/T$, we have

$$\begin{aligned}
H_{\pm a}(x) &= \frac{e^{\frac{-F(1\pm 1)}{2T(1-k)}}}{D_0}\, e^{\pm v_{a1}(x)} \Bigg\{ \int\limits_x^k \mathrm{d}y\, e^{\mp v_{a1}(y)} + \int\limits_k^1 \mathrm{d}y\, e^{\mp v_{b1}(y)} + \int\limits_1^{x+1} \mathrm{d}y\, e^{\mp v_{a2}(y)} \Bigg\}, \\
H_{\pm b}(x) &= \frac{e^{\frac{-F(1\pm 1)}{2T(1-k)}}}{D_0}\, e^{\pm v_{b1}(x)} \Bigg\{ \int\limits_x^1 \mathrm{d}y\, e^{\mp v_{b1}(y)} + \int\limits_1^{k+1} \mathrm{d}y\, e^{\mp v_{a2}(y)} + \int\limits_{k+1}^{x+1} \mathrm{d}y\, e^{\mp v_{b2}(y)} \Bigg\}. 
\end{aligned} \tag{4.19}$$

Performing integration in Eqs. (4.19), we obtain

$$
\begin{aligned}
H_{\pm a}(x) &= \frac{\varphi_0}{a} + g\,\varphi_a \exp\left(\frac{a\,[\mp 2x - k(1\mp 1)]}{2T}\right)\,, \\
H_{\pm b}(x) &= -\frac{\varphi_0}{b} + g\,\varphi_b \exp\left(\frac{b\,[\pm 2(x-1) + (1-k)(1\pm 1)]}{2T}\right)\,,
\end{aligned}
\tag{4.20}
$$

with the notations

$$
g = \frac{1}{a} + \frac{1}{b}\,, \tag{4.21}
$$

$$
\begin{aligned}
\varphi_a &= \exp\left(\frac{1-F}{T}\right) - 1\,, \\
\varphi_b &= 1 - \exp\left(-\frac{1-(1-F)k}{T(1-k)}\right)\,.
\end{aligned}
\tag{4.22}
$$

Substituting the functions $H_{\pm a,b}(x)$ from Eqs. (4.20) into (4.17) and (4.18), we have after integration

$$
Z = \left(\frac{k}{a} - \frac{1-k}{b}\right)\varphi_0 + Tg^2\varphi_a\,\varphi_b\,, \tag{4.23}
$$

$$
\begin{aligned}
Y \;=\; & \left(\frac{k}{a^3} - \frac{1-k}{b^3}\right)\varphi_0^3 + 3T\left(\frac{1}{a^3} + \frac{1}{b^3}\right) g\,\varphi_0^2\,\varphi_a\,\varphi_b \\
& + \frac{1}{2}Tg^2\varphi_0\left[\frac{1}{a^2}\,\varphi_a^2\,\tilde{\varphi}_b - \frac{1}{b^2}\,\varphi_b^2\,\tilde{\varphi}_a\right] \\
& + 2g^2\varphi_0\left[\frac{k}{a}\,\varphi_a^2(1-\varphi_b) - \frac{1-k}{b}\,\varphi_b^2(1+\varphi_a)\right] \\
& + Tg^3\left[\frac{1}{a}\,\varphi_a^3\,\varphi_b(1-\varphi_b) + \frac{1}{b}\,\varphi_b^3\,\varphi_a(1+\varphi_a)\right],
\end{aligned}
\tag{4.24}
$$

where

$$
\begin{aligned}
\tilde{\varphi}_a &= \exp\left(\frac{2(1-F)}{T}\right) - 1\,, \\
\tilde{\varphi}_b &= 1 - \exp\left(-\frac{2[1-(1-F)k]}{T(1-k)}\right)\,.
\end{aligned}
\tag{4.25}
$$

By that we have derived the exact algebraic expressions for the current $\langle \dot{x} \rangle$, the diffusion coefficient $D$, and the Péclet factor Pe.

### 4.3.2 Asymptotic limits and particular cases

In this Section we will examine the asymptotic limits and essential particular cases on the basis of the analytical formulas derived.

(I) In the absence of tilt ($F = 0$), Eqs. (4.16) and (4.22) reduce to

$$\varphi_0 = 0\,, \qquad \varphi_a = e^{1/T} - 1\,, \qquad \varphi_b = 1 - e^{-1/T}, \tag{4.26}$$

and from Eqs. (4.13), (4.23), and (4.24) one obtains

$$D = \frac{1}{2T\,[\cosh(1/T) - 1]}\,. \tag{4.27}$$

This expression is as a special case of the general formula of the diffusion coefficient for arbitrary unbiased periodic potential [52] (see Eq. (3.30)). It is to be noticed that for $F = 0$ the coefficient of diffusion becomes independent of the asymmetry parameter $k$.

(II) In the high temperature limit, one can take into account only the first order terms in the expansions of the exponents in Eqs. (4.16) and (4.22). Then

$$\varphi_0 \approx \frac{F}{T(1-k)}, \qquad \varphi_a \approx \frac{1-F}{T}, \qquad \varphi_b \approx \frac{1-(1-F)k}{T(1-k)}\,, \tag{4.28}$$

and

$$H_{\pm a,b} = T^{-1}\,, \qquad Z = T^{-1}\,, \qquad Y = T^{-3}. \tag{4.29}$$

The diffusion coefficient, current, and Péclet factor now become

$$D = T\,, \tag{4.30}$$

$$\langle \dot{x} \rangle = \frac{F}{1-k}\,, \tag{4.31}$$

$$\mathrm{Pe} = \frac{F}{T(1-k)}\,. \tag{4.32}$$

(III) Under the conditions $F \gg 1$ and $F/T \gg 1$, it is valid that

$$\varphi_0 \approx -\varphi_a \approx \varphi_b \approx 1\,, \qquad a \approx -b \approx \frac{F}{1-k}\,, \tag{4.33}$$

and

$$H_{\pm a,b} = \frac{1-k}{F}\,, \qquad Z = \frac{1-k}{F}\,, \qquad Y = \left(\frac{1-k}{F}\right)^3\,. \tag{4.34}$$

As a result, the expressions for $D$, $\langle \dot{x} \rangle$, and Pe coincide with Eqs. (4.31)-(4.32). Thus, at high temperatures and at large values of tilting force, the transport properties of Brownian particles are the same.

(IV) If $F < 1$ and $(1-F)/T \gg 1$, we have the following asymptotic limits:

$$\varphi_b \approx \tilde{\varphi}_b \approx 1\,, \qquad \varphi_a \approx e^{(1-F)/T} \gg 1\,, \qquad \tilde{\varphi}_a \approx e^{2(1-F)/T} = \varphi_a^2\,. \tag{4.35}$$

Then Eqs. (4.17) and (4.18) with (4.20) yield

$$Z = Tg^2 e^{(1-F)/T}\,, \tag{4.36}$$

$$Y = \frac{T}{2}\, g^3\, e^{2(1-F)/T} [(a^{-1} - b^{-1})\, \varphi_0 + 2(a^{-1} e^{-F/(1-k)T} + b^{-1})]\,, \tag{4.37}$$

and

$$D = \frac{2 - \varphi_0}{2Tg^2\, e^{(1-F)/T}}\,, \tag{4.38}$$

$$\langle \dot{x} \rangle = \frac{\varphi_0}{Tg^2\, e^{(1-F)/T}}\,, \tag{4.39}$$

$$\mathrm{Pe} = \frac{2\varphi_0}{2-\varphi_0} = 2\tanh\frac{F}{2T(1-k)}\,, \tag{4.40}$$

(cf.also Ref. [14]). If, additionally, the condition $F/T(1-k) \gg 1$ is fulfilled, it is valid that $e^{-F/T(1-k)} \approx 0$ and $\varphi_0 \approx 1$. Consequently, in the present case we have $2D = \langle \dot{x} \rangle$ and $\mathrm{Pe} = 2$. This indicates that an extremely exact stabilization of the level of coherence of Brownian transport occurs in this region of parameters.

(V) At the critical tilt ($F = 1$), it is valid that

$$\begin{aligned} H_{\pm a}(x) &= \frac{\varphi_0}{a} + \frac{1-k}{T}\exp\left(\frac{a\left[\mp 2x - k(1\mp 1)\right]}{2T}\right)\,, \\ H_{\pm b}(x) &= \frac{\varphi_0}{a} + \frac{1-k}{T}\exp\left(-\frac{ak}{T}\right) + \frac{\varphi_0\left[\pm 2(x-1) + (1-k)(1\pm 1)\right]}{2T}\,, \end{aligned} \tag{4.41}$$

whereas in the low-temperature limit Eqs. (4.13)-(4.18) and (4.41) yield

$$D = \frac{2T}{3(1-k)^2}\,, \tag{4.42}$$

$$\langle \dot{x} \rangle = \frac{2T}{(1-k)^2}\,, \tag{4.43}$$

$$\mathrm{Pe} = 3\,. \tag{4.44}$$

We observe that, for $F = 1$ the Péclet factor is constant and depends neither on the temperature nor on the asymmetry parameter.

### 4.3.3 Non-monotonic behavior of diffusion

We studied the behavior of the diffusion coefficient, current and Péclet factor for certain values and limits of temperature and tilting force. We now discuss the general dependencies of the transport characteristics on the system parameters.

The expression of the diffusion coefficient as a function of tilting force $F$ and temperature $T$ is given by Eqs. (4.13), (4.23), and (4.24). The diffusion coefficient as a

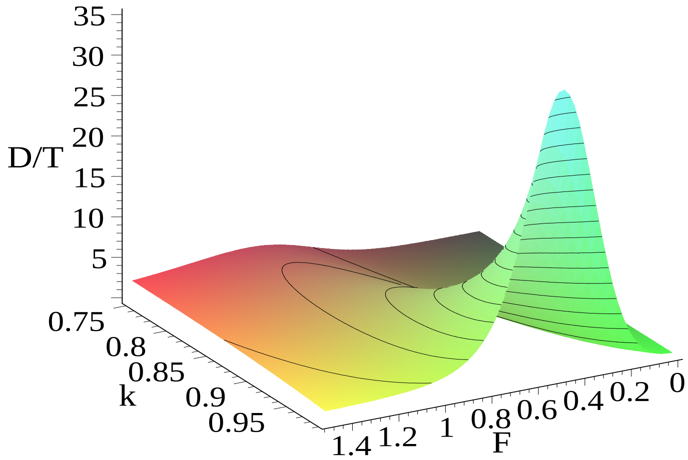


Figure 4: Diffusion coefficient *vs* tilting force $F$ and the potential asymmetry parameter $k$ at fixed $T = 0.1$.

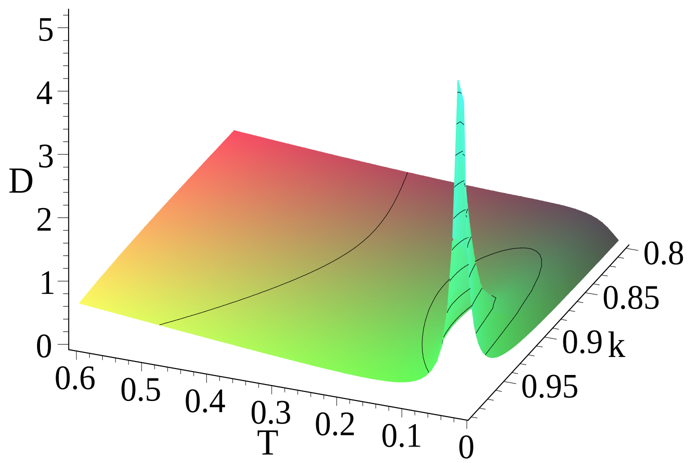


Figure 5: Diffusion coefficient *vs* the temperature $T$ and the potential asymmetry parameter at fixed $F = 0.95$.

function of $F$ reveals a qualitatively similar behavior to that found in Refs. [15], exhibiting a resonant-like maximum if the temperature is sufficiently low. This effect is strongly influenced by the shape of the periodic potential, as illustrated in Fig. 4. For positive bias ($F > 0$), the increase of the value of $k$ favors the amplification of diffusion compared to free thermal diffusion.

The behavior of the diffusion coefficient as a function of temperature is similar to that observed in Ref. [14] (see also Ref. [16, 17]): There exists a maximum of $D(T)$, which is followed by a minimum (see Fig. 5). The existence of the suppression in $D(T)$ is attributed to the competition between two time scales: Noise driven escape over potential barrier from the minima along the bias, and the second time scale being the relaxation into the next potential well from the barrier top [14]. The second time scale is weakly dependent on noise intensity and has a small variance as opposed to the first one. When the second time scale dominates over the first one, it is expected to result in suppression of diffusion coefficient as a function of temperature (see Ref. [14]). The influence of the potential shape on the diffusion coefficient $D(T)$ is analogous to the one on $D(F)$: The peak of $D(T)$ becomes rapidly narrower and higher if $k$ approaches unity.

The analytical properties of the diffusion coefficient as a function of tilting force and temperature at the fixed value of the asymmetry coefficient are summarized by the contour-plot of the surface $D(F, T)$ in Fig. 6. The surface $D(F, T)$ exhibits two stationary points, a maximum and a saddle point, whose coordinates are given in the figure caption. The plot reflects the characteristic features of the non-monotonic behavior of diffusion:

(I) One can observe in Fig. 6 that the function $D(T)|_{F=\mathrm{const}}$ has a maximum and a minimum if $F_A < F < F_B$. However, there exists a limiting value $k_E \approx 0.8285$, inferable from Fig. 5. For $k < k_E$ the maximum and the saddle point of the surface $D(T, F)$ disappear, while $D(T)|_{F=\mathrm{const}}$ is a monotonic function of temperature, the

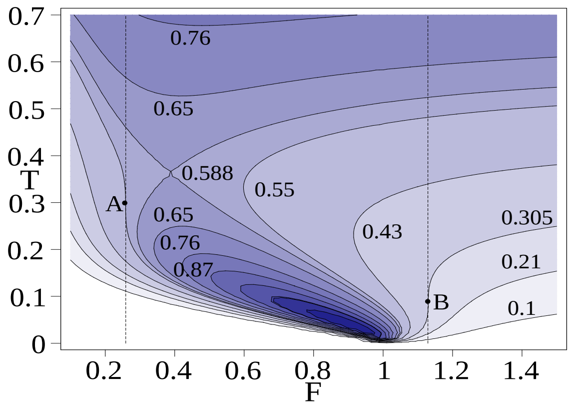


Figure 6: Contour-plot of diffusion coefficient $D = D(F,T)$ for $k = 0.95$. To the maximum and saddle points of $D$ correspond, respectively, the values $F_M \approx 0.9144$, $T_M \approx 0.0364, D_M \approx 1.3086$ and $F_S \approx 0.388, T_S \approx 0.363,\ D_S \approx 0.588$.

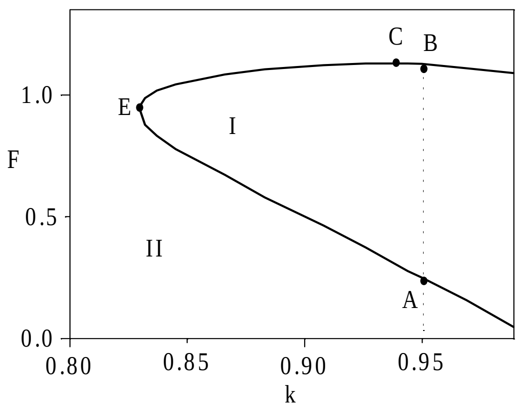


Figure 7: The phase-diagram in the $(k,F)$-plane representing the regions corresponding to the different analytical properties of the diffusion coefficient as a function of temperature: the dependence $D(T)$ is nonmonotonic in the region I, whereas it is monotonic in the region II.

latter property being independent of bias. There also exists a limiting tilting force $F_C \approx 1.1292$. If $F > F_C$, the dependence $D(T)|_{F=\text{const}}$ is monotonic for arbitrary $k$. The situation is summarized in Fig. 7, where one sees that the $(k, F)$-space is divided into two domains where the analytical properties of the diffusion coefficient as a function of temperature are qualitatively different.

(II) Contrary to the dependence $D(T)\,|_{F=\text{const}}$, the function $D(F)\,|_{T=\text{const}}$ has a maximum for all values of asymmetry parameter.

As one can see in Figs. 5 and 6 the suppression of diffusion as a function of temperature is the larger the closer are the asymmetry coefficient $k$ and tilting force $F$ to unity. The effect is maximal, if both of these conditions are fulfilled. The latter fact supports the notion that the counterintuitive phenomenon that increasing noises decreases diffusion relies on the large ratio of relaxation to escape time. However, we remark that the nonmonotonic behavior of $D(T)$ persists in the case of piecewise linear potential also for tilts slightly above the critical value when there is no potential minima.

One can also observe in Fig. 6 that for the potentials with $k > k_E$ the maximal value of $D(F)$ as a function of temperature passes through a minimum, i.e., the amplification of diffusion by bias at lower noise intensity can be larger than at higher temperature.

### 4.3.4 Probabilistic treatment

We now discuss the amplification of diffusion by bias in terms of probability distribution (3.26). Figure 8 represents (in terms of the dimensionless parameters) the probability distributions characteristic of various diffusion levels depending on the tilting force. Figure 8-a illustrates the situation, where particles are mainly localized around the minima of the potential and transport is strongly suppressed. Diffusion

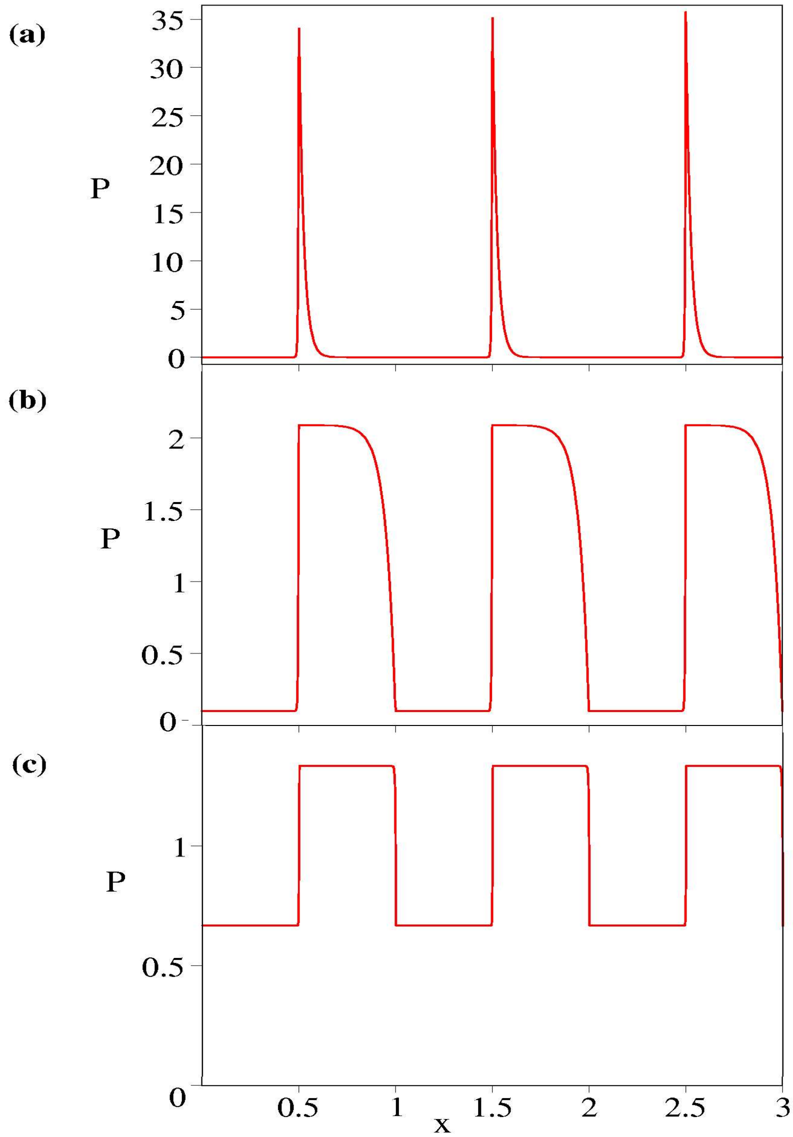


Figure 8: Probability density $P(x)$ for the temperature $T = 0.01$ and asymmetry parameter $k = 0.5$: (a) $F = 0.8$; (b) $F = 1.1$; (c) $F = 3$.

is essentially weaker in comparison with free diffusion: $D/T \sim 10^{-6}$. The probability distribution shown in Fig. 8-b corresponds to the case where the diffusion is approximately maximal ($D/T = 3.5$) for the chosen values of temperature and asymmetry coefficient. In this case the regions with a large probability are separated by the domains where the probability is much smaller, however, large enough to allow the entrance of a sufficient number of particles into these domains. As a result, a channel of hopping-like transport is formed, leading to the enhancement of diffusion with respect to free diffusion. The further increase of the tilting force $F$ makes the probability distribution still more homogeneous, as seen in Fig. 8-c, and the diffusion approaches the free diffusion limit ($D/T = 1.3$ for the values of the parameters used in Fig. 8-c).

Consequently, the amplified diffusion in the tilted periodic potential is characterized by the specific inhomogeneous probability distribution with spatially alternating domains of high and low probability. The occurrence of a maximum in the of dependence $D(T)$ can be understood in a similar way.

### 4.3.5 Non-monotonic behavior of coherence: Optimization of transport

In Fig. 9 the curves of the Péclet factor *vs* temperature for various values of $k$ and $F$ are depicted. The function $\mathrm{Pe}(T)$ passes through a maximum (curves 1-5) for $F < F_c$, which is also present slightly above the critical tilt (curve 6). With a further increase of $F$, the maximum of $\mathrm{Pe}(T)$ disappears.

As seen in Fig. 9, the optimal level of Brownian transport, determined by the maximal value of the Péclet number, is sensitive to the shape of periodic potential: at $F < F_c$ the optimal level of transport rises with an increase in $k$. At the same time, the larger values of $k$ make a minimum of $D(T)$, which follows a maximum of $D(T)$ at a higher value of temperature, deeper (the effect can be anticipated in Fig. 5). Figure 10 shows that the enhancement of the coherence of Brownian motion in a

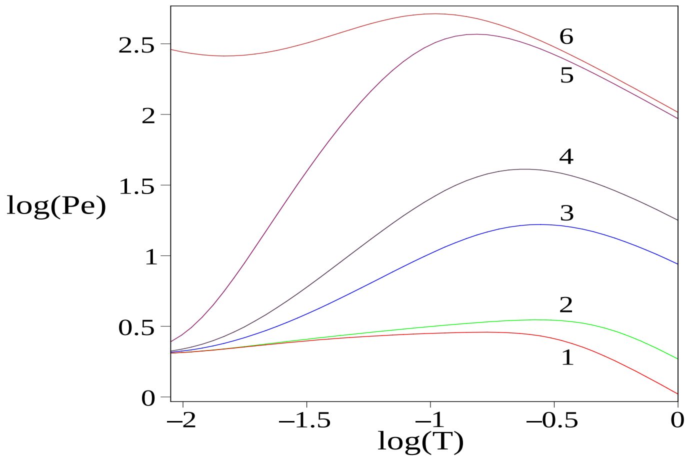


Figure 9: Péclet factor $\log_{10}(\mathrm{Pe})$ *versus* temperature $\log_{10}(T)$ for various values of the potential asymmetry coefficient at $F = 0.95$ (curves 1-5) and $F = 1.05$ (curve 6). (1) $k = 0.1$, (2) $k = 0.5$, (3) $k = 0.9$, (4) $k = 0.95$, curves 5, 6: $k = 0.99$.

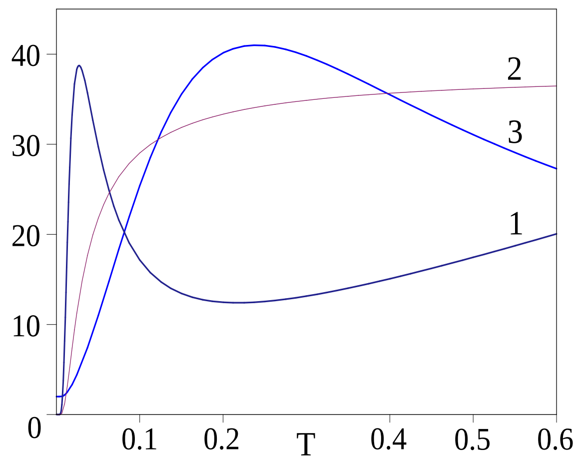


Figure 10: Diffusion coefficient, current, and Péclet factor *vs* temperature for $k = 0.95$, $F = 0.95$: (1) $30 \times D$; (2) $2 \times \langle \dot{x} \rangle$; (3) Pe.

certain region of temperature is associated with the suppression of diffusion by the same factor (collate also Figs. 9 and 5).

### 4.3.6 Correlation between the enhancement of diffusion and stabilization of coherence

With regard to the simultaneous enhancement of diffusion and current, caused by the force $F$, with respect to an untilted system, the relation between $D$ and $\langle \dot{x} \rangle$ is of interest. One can expect that such a relationship reflects some intrinsic features of the mutual influence between diffusion and current driven by the tilt merely at lower temperatures, when the initial suppression of both components of Brownian transport by periodic potential is stronger.

The comparative plot of $D$ and Pe *vs* $F$ is presented in Figs. 11 and 12. One can see that the function Pe$(F)$ has a point of inflection which turns into a wide plateau at lower temperatures. For values of $F$, from zero up to the end of the plateau, the behavior of Pe$(F)$ is described with great accuracy by Eq. (4.40). As the temperature grows, the plateau gradually reduces until disappears and the Péclet factor becomes monotonically increasing.

We emphasize that the domain where Pe $= 2$ coincides with the domain where the increase of diffusion coefficient as a consequence of the tilting is most rapid. Consequently, in the region of parameters, where the substantial acceleration of diffusion (and also current) occurs, the directed transport and diffusion are very exactly synchronized. Note that the stabilization of the coherence level at the value of the Péclet factor Pe $= 2$ is a characteristic feature of Poissonian process [1] such as the Poisson enzymes in kinesin kinetics [62, 64, 65]. The location of the end of this region at larger values of $F$ is quite insensitive to the shape of the periodic potential, as seen in Fig. 12, and is located approximately at critical tilt $F_c$.

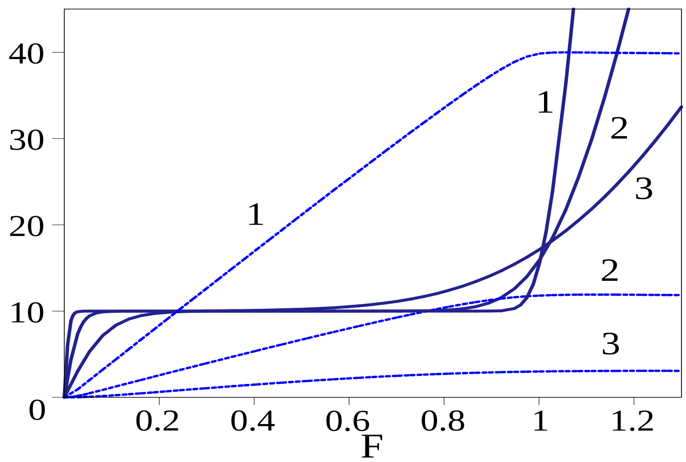


Figure 11: Comparison between the Péclet factor Pe and diffusion coefficient $D$ as a function of tilting force $F$ for various temperatures at fixed $k = 0.5$. Solid lines: $5 \times$ Pe, dashed lines: $\log_{10}[D(F)/D(0)]$. Curves 1: $T = 0.01$, curves 2: $T = 0.03$, curves 3: $T = 0.09$.

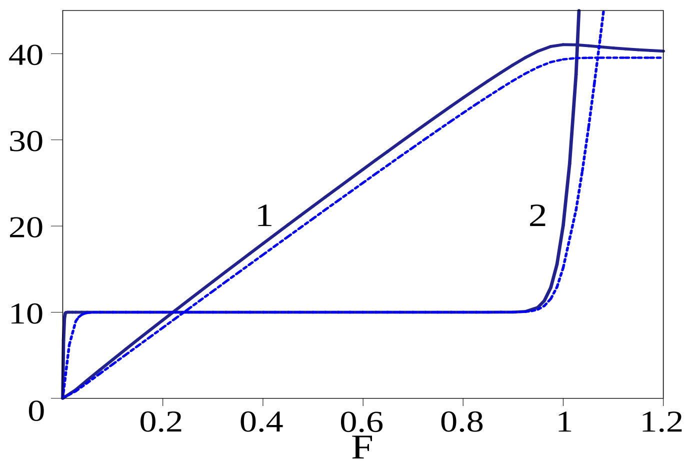


Figure 12: Comparison between the Péclet factor Pe and diffusion coefficient $D$ as a function of tilting force $F$ for $k = 0.1$ (dashed lines) and $k = 0.9$ (solid lines) at fixed $T = 0.01$. Curves 1: $\log_{10}[D(F)/D(0)]$, curves 2: $5 \times$ Pe.

It is remarkable that, as a result of the interplay of periodic potential, bias and white noise, there exists an exact correlation between the acceleration of diffusion, induced by the tilting force, and the stabilization of the coherence level of Brownian motion. It seems that this phenomenon is quite universal and manifests itself for an arbitrary periodic potential in situations where initially strongly suppressed transport is enhanced by bias, which generates significant amplification of diffusion in comparison with free diffusion.

### 4.3.7 Conclusion

Acceleration of diffusion turns out to be very sensitive to the shape of the piecewise linear potential. It is shown that large values of the asymmetry parameter $k$ favor the amplification of diffusion by means of biased potential and temperature in comparison with free thermal diffusion. This can be understood as a result of the formation of probability distribution with spatially alternating regions of specifically balanced high and low probability. The necessary and sufficient conditions for the non-monotonic behavior of the diffusion coefficient as a function of temperature are established. We also have shown a possibility to attain a counterintuitive situation, where at lower noise intensities the maximal of the diffusion coefficient $D(F)$ can be larger than at higher noise intensities.

We have shown that the shape of the potential has a great influence also on the coherence level in a certain region of temperature. However, at low temperatures and for the subcritical tilt, the coherence of Brownian transport is demonstrated to have the value $\mathrm{Pe} = 2$ practically independent of the potential shape. The domain, where the Péclet factor exhibits the plateau, coincides with the domain where the enhancement of diffusion coefficient is maximal. Consequently, in the region of parameters where substantial acceleration of diffusion occurs, the current and diffusion are exactly synchronized.

## 4.4 Diffusion and coherence in tilted piecewise linear double-periodic potentials

### 4.4.1 Analytic computations

The analytical results for the diffusion coefficient, current and Péclet factor are obtained in a way similar to the calculations for the simple sawtooth potential. In the case of double-periodic potential, in Eqs. (4.13)-(4.15) the quantities $Z$ and $Y$ now have the form

$$Z = \int_0^{k_1} \mathrm{d}x\, H_{-a}(x) + \int_{k_1}^{k_2} \mathrm{d}x\, H_{-b}(x) + \int_{k_2}^{k} \mathrm{d}x\, H_{-c}(x) + \int_{k}^{1} \mathrm{d}x\, H_{-d}(x)\,, \tag{4.45}$$

$$\begin{aligned} Y &= \int_0^{k_1} \mathrm{d}x\, H_{+a}(x)\, H_{-a}^2(x) + \int_{k_1}^{k_2} \mathrm{d}x\, H_{+b}(x)\, H_{-b}^2(x) \\ &\quad + \int_{k_2}^{k} \mathrm{d}x\, H_{+c}(x)\, H_{-c}^2(x) + \int_{k}^{1} \mathrm{d}x\, H_{+d}(x)\, H_{-d}^2(x)\,. \end{aligned} \tag{4.46}$$

Here

$$\begin{aligned} H_{\pm a}(x) &= \frac{e^{\frac{-F(1\pm 1)}{2T(1-k)}}}{D_0}\, e^{\pm v_{a1}(x)} \Bigg\{ \int_x^{k_1} \mathrm{d}y\, e^{\mp v_{a1}(y)} + \int_{k_1}^{k_2} \mathrm{d}y\, e^{\mp v_{b1}(y)} \\ &\quad + \int_{k_2}^{k} \mathrm{d}y\, e^{\mp v_{c1}(y)} + \int_{k}^{1} \mathrm{d}y\, e^{\mp v_{d1}(y)} + \int_{1}^{x+1} \mathrm{d}y\, e^{\mp v_{a2}(y)} \Bigg\}\,, \\ H_{\pm b}(x) &= \frac{e^{\frac{-F(1\pm 1)}{2T(1-k)}}}{D_0}\, e^{\pm v_{b1}(x)} \Bigg\{ \int_x^{k_2} \mathrm{d}y\, e^{\mp v_{b1}(y)} + \int_{k_2}^{k} \mathrm{d}y\, e^{\mp v_{c1}(y)} \\ &\quad + \int_{k}^{1} \mathrm{d}y\, e^{\mp v_{d1}(y)} + \int_{1}^{k_1+1} \mathrm{d}y\, e^{\mp v_{a2}(y)} + \int_{k_1+1}^{x+1} \mathrm{d}y\, e^{\mp v_{b2}(y)} \Bigg\}\,, \\ H_{\pm c}(x) &= \frac{e^{\frac{-F(1\pm 1)}{2T(1-k)}}}{D_0}\, e^{\pm v_{c1}(x)} \Bigg\{ \int_x^{k} \mathrm{d}y\, e^{\mp v_{c1}(y)} + \int_{k}^{1} \mathrm{d}y\, e^{\mp v_{d1}(y)} \end{aligned}$$

$$
\begin{aligned}
& + \int_{1}^{k_1+1} \mathrm{d}y \, e^{\mp v_{a2}(y)} + \int_{k_1+1}^{k_2+1} \mathrm{d}y \, e^{\mp v_{b2}(y)} + \int_{k_2+1}^{x+1} \mathrm{d}y \, e^{\mp v_{c2}(y)} \Bigg\}, \\
H_{\pm d}(x) \;=\; & \frac{e^{\frac{-F(1\pm 1)}{2T(1-k)}}}{D_0} \, e^{\pm v_{d1}(x)} \Bigg\{ \int_{x}^{1} \mathrm{d}y \, e^{\mp v_{d1}(y)} + \int_{1}^{k_1+1} \mathrm{d}y \, e^{\mp v_{a2}(y)} \\
& + \int_{k_1+1}^{k_2+1} \mathrm{d}y \, e^{\mp v_{b2}(y)} + \int_{k_2+1}^{k+1} \mathrm{d}y \, e^{\mp v_{c2}(y)} + \int_{k+1}^{x+1} \mathrm{d}y \, e^{\mp v_{d2}(y)} \Bigg\}. \qquad (4.47)
\end{aligned}
$$

The explicit algebraic expressions for $Z$ and $Y$ are revealed in Appendix A.

### 4.4.2 Diffusion

We first emphasize that the general character of the transport process is, compared to the corresponding simple sawtooth case, determined by the value of $F_{ce}$, and thus for a fixed $k$ by the differences $\Delta A$ and $\Delta k$. The values of single parameters $k_1, k_2, A_1, A_2$ are of no importance, while the differences $\Delta A$ and $\Delta k$ are crucial, even if the values of $F_{ce}$, determined by them, are the same.

A double-periodic potential gives a possibility to favor or suppress the maximal value of the diffusion coefficient $D(F)$, compared to the case of the simple sawtooth potential. The situation is illustrated in Fig. 13. In the case $F_{ce} < F_c$ the maximal value of $D(F)$ is decreased due to the additional potential minima. The decrease is, at fixed $k$ and $\Delta A$, the largest if $F_{ce} = F_c$. For $F_{ce} > F_c$ diffusion starts to increase. If $F_{ce}$ is larger than the value of the tilting force, which corresponds to the maximum of $D(F)$ in the case of the simple sawtooth potential, then the maximal value of diffusion increases due to the extra trap.

Henceforth our main interest will be focused on the potentials with $F_{ce} > F_c$, which provide new phenomena with respect to the case of simple periodic potentials. The case $F_{ce} < F_c$ does not differ, if $F \to F_c$, much from the case of the simple sawtooth potential. However, we remark that in biological systems the potentials, for which

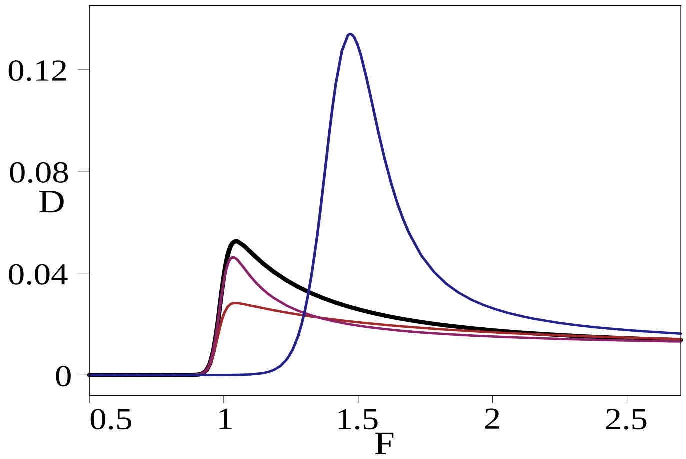


Figure 13: The enhancement and suppression of the diffusion coefficient, compared to the simple sawtooth potential, due to the additional trap. $T = 0.01$; $k = 0.6$, $\Delta A = 0.45$. In the decreasing order of the maximal values of $D(F)$: (1) $F_{ce} = 1.5$; (2) simple sawtooth potential; (3) $F_{ce} = 0.5$; (4) $F_{ce} = F_c = 1$.

$F_{ce} < F_c$, often play a role [66].

In Fig. 14 we have plotted the diffusion coefficient *vs* tilting force at different values of temperature, for a potential for which $F_{ce} > F_c$ [2]. This figure highlights a counterintuitive phenomenon: at lower noise intensities, the maximal value of the diffusion coefficient $D(F)$ can be bigger than at higher noise intensities (compare curves 2, 3 and 4 with each other, or 1 with 4, or 2 with 5). At low and high values of temperature the situation is back to usual (compare curves 1 with 2, and 4 with 5). As one can see in Fig. 6 the analogous situation is observable for the simple sawtooth potential in the case $k > k_E$. However, the additional potential maximum per period with $F_{ce} > F_c$ allows one to obtain the effect also for the potentials with asymmetry parameter $k < k_E$. The general behavior of the diffusion coefficient

[2] If not marked otherwise in the figure capture, we henceforth calculate all the graphics for the same values of potential parameters: $k_1 = 0.4$, $k_2 = 0.5$, $k = 0.6$, $A_1 = 0.55$, $A_2 = 1$; $F_{ce} = 1.8$.

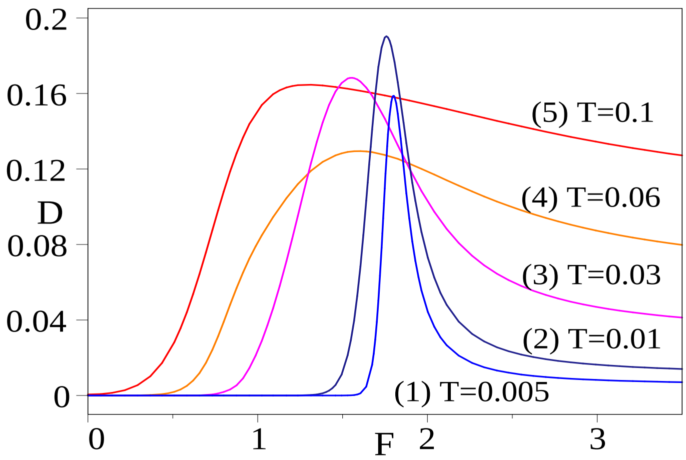


Figure 14: Diffusion coefficient $D(F)$ for different values of temperature. Potential parameters: $k_1 = 0.4$, $k_2 = 0.5$, $k = 0.6$, $A_1 = 0.55$, $A_2 = 1$; $F_{ce} = 1.8$.

$D(T, F)$ is the same as one can see in Fig. 6, for the potential with one minimum per period.

Figure 15 represents the dependence $D(F)$ in the case of the same potential as used in Fig. 14, but in a logarithmic scale. In this plot one can distinguish two acceleration rates for the diffusion. The two rates are the more different, the lower the noise intensity, and associate with the two Poissonian processes (the latter fact will be discussed in more detail in next Subsection). Thereby the Poissonian process in the first region coincides with the one which takes place in the corresponding simple sawtooth potential. The picture for the current is similar.

The presence of two potential barriers may lead one to think that there can be two maxima of the diffusion coefficient *vs* tilting force, but in practice such a situation is difficult to attain. Nevertheless, for a certain type of potential shape it is possible to obtain a situation, for which the diffusion coefficient $D(F)$ possesses two maxima and passes a considerable minimum under the critical tilt [3] (see Fig. 16). The

[3] Actually there exists also another minimum in the region of small tilting values. Such a

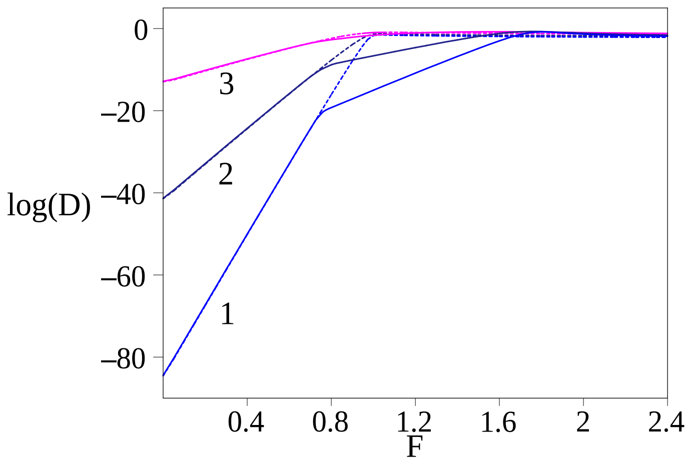


Figure 15: Diffusion coefficient $\log_{10}[D(F)]$ for different noise intensities. Solid lines: The potential parameters are the same as in Fig. 3; (1) $T = 0.005$; (2) $T = 0.01$; (3) $T = 0.03$. Dashed lines: Diffusion coefficients for the sawtooth potential with asymmetry parameter $k = 0.6$ at the same temperatures.

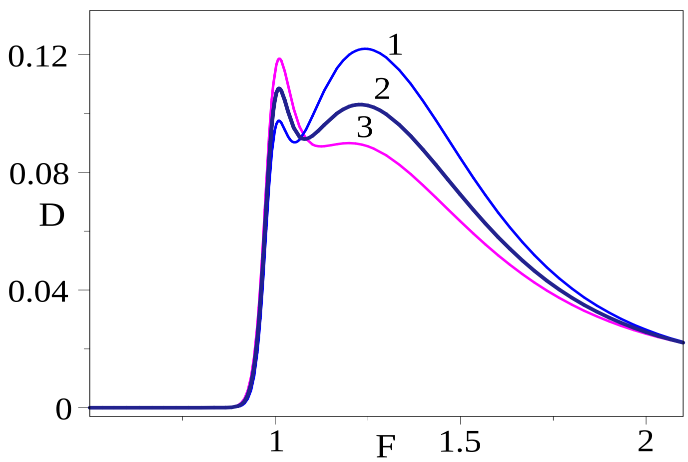


Figure 16: The existence of two maxima for diffusion coefficient *vs* tilting force for different noise intensities: (1): $T = 0.0095$; (2): $T = 0.01$; (3): $T = 0.0105$. The potential parameters are: $k_1 = 0.79$, $k_2 = 0.8$, $k = 0.81$, $A_1 = 0.888$, $A_2 = 1$.

minimum of $D(F)$ is the deepest in the temperature region where the amplification of diffusion is minimal and the maxima of $D(F)$ are equal. At higher and lower temperatures one of the maxima starts to dominate and the other one to decrease. To obtain two maxima in the dependence of $D(F)$ a small but sharp additional potential barrier is needed, which is followed by a steep fall. However, the situation is extremely sensitive to the potential parameters and to the noise intensity.

### 4.4.3 Coherence of motion

In the case of simple sawtooth potential we showed that at low temperatures and for subcritical tilt the coherence level stabilizes at the value of Péclet number $\mathrm{Pe}(F) = 2$. The situation corresponds to the case when particles are mainly localized around the potential minima and transport can be described with great accuracy by the Poissonian hopping process.

Considering the double-periodic potentials, the average distribution of Brownian particles can change at low temperatures drastically for different values of the subcritical tilting force. For the potentials with $F_{ce} > 1$ there exists a threshold value of the tilting force,

$$F_0 = \frac{(1-\Delta A)(1-k)}{1-k-\Delta k}\,, \tag{4.48}$$

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 *vs* tilting force is realized through two different Poissonian processes: The first one takes place if $F < F_0$, while the second one if $F > F_0$. As seen in Fig. 17, the two regions of the

suppression of diffusion by a weak external force is obtainable as well for the simple sawtooth potential with $k > 0.5$. However, the discussion of this effect is not included into the present thesis.

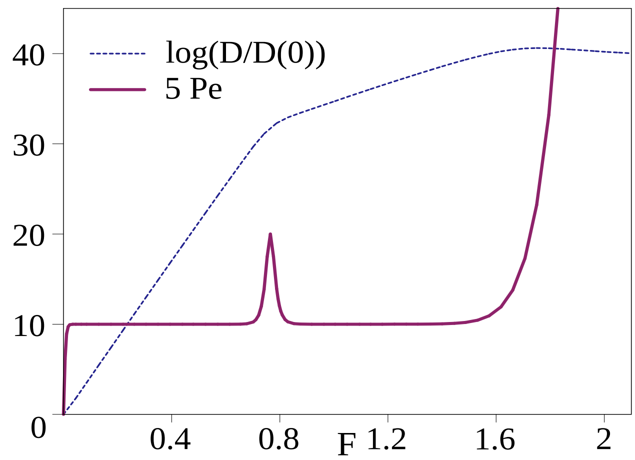


Figure 17: Comparison between diffusion coefficient and Péclet number as a function of the tilting force. Dashed line: $\log_{10}[D(F)/D(0)]$; Solid line: $5 \times \mathrm{Pe}$. Temperature $T = 0.01$.

acceleration of diffusion in Fig. 15 correspond to these different Poisson processes. In the region of crossover between the two regimes of the enhancement of diffusion, the Péclet number passes through a sharp maximum (a minimum in randomness parameter) with the characteristic value $\mathrm{Pe} = 4$ ($r = 1/2$).

The observed enhancement of coherence — decrease of randomness — 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 (see Fig. 18). 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. In Fig. 18 one can also see that the tilting force $F_0$ lies approximately in the beginning of the domain of crossover ($F_0 = 0.733$).

For the existence of the extremum in the coherence of Brownian motion *vs* tilt, the condition $F_{ce} > 1$ must be satisfied. The tilting force $F_0$ has a physical meaning

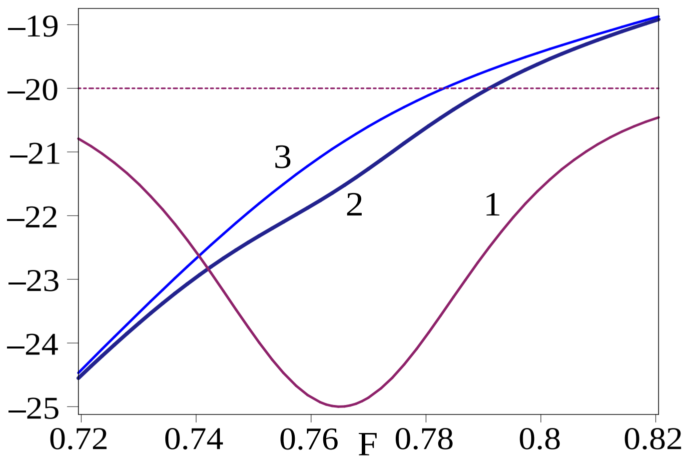


Figure 18: The appearance of the minimum in the randomness parameter $r(F)$ in the region of the crossover. The curves represent the randomness parameter, diffusion coefficient and current *vs* tilting force at $T = 0.01$: (1) $10 \times (r - 3)$; (2) $\ln(2D)$; (3) $\ln(\langle \dot{x} \rangle)$; the dashed line corresponds to the coherence level $r = 1$.

only if the latter inequality is fulfilled, having the value in the range $0 < F_0 < 1$. This circumstance follows [4] from Eq. (4.48) together with Eq. (4.8) for $F_{ce}$ which lead to the relation

$$(1 - F_0) = \frac{\Delta k}{1 - k - \Delta k} \left( F_{ce} - 1 \right). \tag{4.49}$$

If $F_{ce} < 1$, the Péclet number $\mathrm{Pe}(F)$ does not have a maximum [5]. On the other hand, if $F_0 < 1$ is sufficiently close to unity, the peak of coherence merges into the region where the motion can no longer be described as the Poissonian process and $\mathrm{Pe}(F)$ increases monotonically. In particular, such a case is actual for the potentials for which the diffusion coefficient $D(F)$ possesses two maxima.

[4]Note that for $F_{ce} > 1$ the condition $\Delta k < 1 - k$ must be always fulfilled as one can see from Eq. (4.8).

[5]The inequality $F_{ce} < 1$ is valid always if $\Delta k > 1 - k$ (see Eq. (4.8)) and then one can see from Eq. (4.48) that $F_0 < 0$. However, condition $F_{ce} < 1$ can be satisfied also for $\Delta k < 1 - k$ which

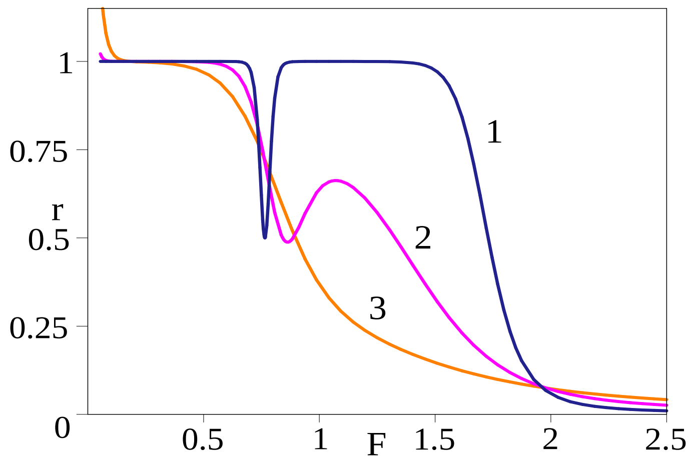


Figure 19: Randomness parameter $r$ *vs* tilt $F$ for different noise intensities: (1) $T = 0.01$; (2) $T = 0.03$; (3) $T = 0.06$.

With the rise of temperature the peak of the coherence disappears. We have illustrated the situation in Fig. 19 for the randomness parameter. At higher temperature the posterior part of the plateau of randomness parameter diminishes and the minimum broadens, and finally the randomness decreases and the coherence increases monotonically.

For the simple sawtooth potential we demonstrated the possibility to obtain the existence of a maximum in the Péclet number *vs* temperature (cf. Ref. [14]), in connection with the minimum in the diffusion coefficient, for increasing noise intensity. In Ref. [16] it is pointed out that for a homogeneous system the Péclet number can show a maximum, although neither the diffusion coefficient nor the average current density shows an extremum. The present model allows us to observe for different tilts both the phenomena as one can see in Fig. 20 (the situation is actually valid also for the simple sawtooth potential, however, in Fig. 9 it is intricate to understand). Furthermore, as one can see in Fig. 21, in the region of static external force, where

yield on the basis of Eq. (4.49) $F_0 > 1$.

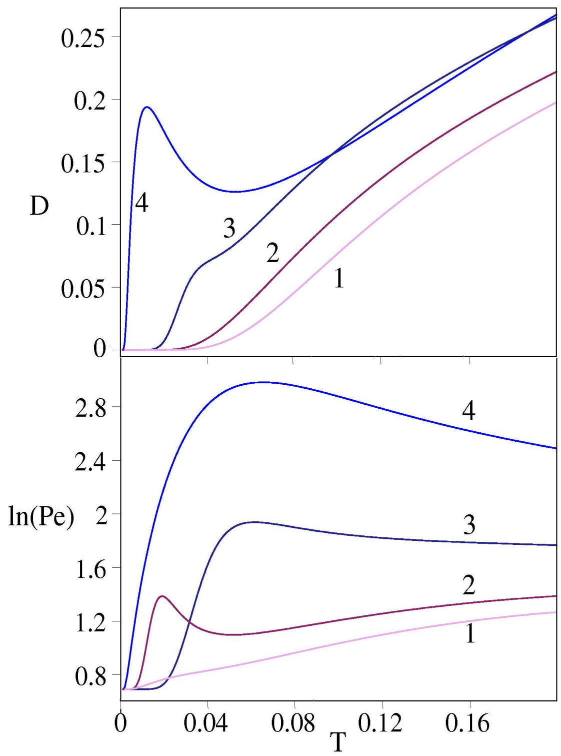


Figure 20: Diffusion coefficient $D$ and ln(Pe) *vs* temperature for different tilts: (1) $F = 0.7$; (2) $F = 0.8$; (3) $F = 1.1$; (4) $F = 1.75$.

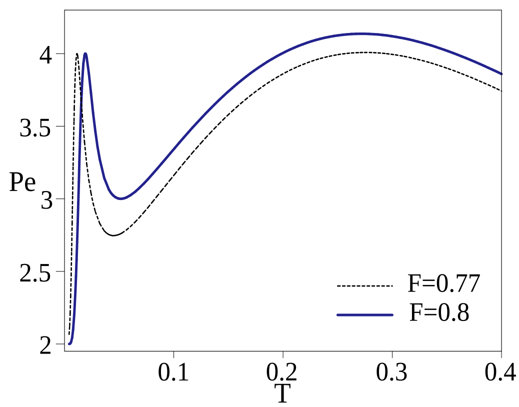


Figure 21: The existence of two maxima in Pe *vs* $T$.

Pe($F$) exhibits a maximum (minimum in the randomness factor), the Péclet number *vs* temperature has two maxima, and is extremely sensitive to the noise intensity.

### 4.4.4 Conclusion

The overdamped Brownian motion in tilted double-periodic piecewise linear potentials, significant in biology and condensed matter physics, has been studied. It proves that, due to an additional potential barrier, for certain parameter values, many new effects occur in the transport processes of Brownian particles, in particular if $F_{ce} > F_c$.

The general dependence of the diffusion coefficient *vs* tilting force obeys as a rule the typical behavior found for simple sawtooth potential. However, in the present case, the acceleration of diffusion is characterized by two regions, related to the two potential barriers and corresponding different Poissonian processes. In the domain of crossover between these two regimes the level of coherence of transport passes through a sharp maximum. Furthermore, for a certain type of potentials, the effective diffusion coefficient $D(F)$ can have two maxima.

# 5 Summary

In the present thesis we have carried out a comprehensive investigation of the overdamped Brownian motion in tilted periodic potentials with one and two minima per period in the presence of white thermal noise. We have done this by using piecewise linear potentials, which can be considered as a first approximation of the shape of arbitrary potentials. We have derived the explicit algebraic expressions for the diffusion coefficient, particle current, and Péclet number, and analyzed their dependencies on temperature, tilting force, and the shape of the potentials.

We have demonstrated that piecewise linear potentials provide the effects characteristic of the tilted periodic potentials. Furthermore, merely varying the potential shape allows one to obtain also all the phenomena attained in systems with spatially periodic temperature and nonhomogenous dissipation. At the same time the transport properties of particles in the potentials with two minima per period has been shown to exhibit in certain parameter regions also new and qualitatively different features.

It has been shown that the acceleration of diffusion is very sensitive to the shape of the potential. Large values of the asymmetry parameter $k$ in the direction of bias $F$ favor the amplification of diffusion by means of tilted potential and temperature in comparison with free thermal diffusion. In the case of double-periodic potentials the acceleration of diffusion is characterized by two regions with different acceleration rates, while for certain values of potential parameters, the effective diffusion coefficient $D(F)$ can have two maxima. The necessary and sufficient conditions for the non-monotonic behavior of the diffusion coefficient as a function of temperature have been established in the case of simple sawtooth potential.

We have shown that the potential shape has a great influence also on the coherence level in a certain region of temperature. However, at low temperatures and subcritical tilts the coherence of Brownian transport has been demonstrated to have the value $\mathrm{Pe} = 2$, practically independent of the potential shape, and characteristic of Poissonian process. The domain, where the Péclet factor exhibits the plateau, coincides with the domain where the enhancement of diffusion coefficient is maximal. Consequently, in the region of parameters where substantial acceleration of diffusion occurs, current and diffusion are exactly synchronized. In the case of double-periodic potentials the acceleration of diffusion is related to two different Poissonian processes, while in the region of crossover at low temperature a drastic rise of the coherence level takes place. For the values of tilting force, characteristic of the enhancement of the coherence, the Péclet number *vs* noise intensity possesses two maxima.

In conclusion, we have demonstrated that transport processes are extremely sensitive to the value of noise intensity and force. Furthermore, we have shown that also the shape of the periodic potential has a significant influence in determining the character of stochastic transport.

# Appendix

## A Analytical results for double-periodic potential

The analytical results for the diffusion coefficient, current and Péclet factor are given by Eqs. (4.13)-(4.15). Performing the integrations in Eqs. (4.47) one obtains after cumbersome calculations the algebraic expressions for the quantities $Z$ and $Y$, given by Eqs. (4.45) and (4.46), in the case of double-periodic potential:

$$\begin{aligned} Z &= \varphi_0 \left( k_1\, g_{ab} - k_2\, g_{bc} + k\, g_{cd} - \frac{1}{d} \right) + \frac{T}{a}\, S_1 (1-\lambda_1) \\ &+ \frac{T}{b}\, S_2 (1-\lambda_2) - \frac{T}{c}\, S_3 (1-\lambda_3) + \frac{T}{d}\, S_4 (1-\lambda_4)\,, \end{aligned} \tag{A.50}$$

$$\begin{aligned} Y &= \varphi_0^3 \left[ k_1 \left( \frac{1}{a^3} + \frac{1}{b^3} \right) - k_2 \left( \frac{1}{b^3} + \frac{1}{c^3} \right) + k \left( \frac{1}{c^3} + \frac{1}{d^3} \right) - \frac{1}{d^3} \right] \\ &+ T \varphi_0^2 \left[ \frac{(1-\lambda_1)}{a^3} (2S_1 + S_1') + \frac{(1-\lambda_2)}{b^3} (2S_2 + \lambda_2^{-1} S_2') \right. \\ &\left. - \frac{(1-\lambda_3)}{c^3} (2S_3 + S_3') + \frac{(1-\lambda_4)}{d^3} (2S_4 + \lambda_4^{-1} S_4') \right] \\ &+ T \left\{ \frac{(1-\lambda_1)}{a}\, S_1^2 \, [\lambda_1\, S_1' + \frac{\varphi_0}{2a} (1+\lambda_1)] + \frac{1-\lambda_2}{b}\, S_2^2\, [S_2' - \frac{\varphi_0}{2b} (1+\lambda_2)] \right. \\ &\left. - \frac{(1-\lambda_3)}{c}\, S_3^2\, [\lambda_3 S_3' + \frac{\varphi_0}{2c} (1+\lambda_3)] + \frac{(1-\lambda_4)}{d}\, S_4^2\, [S_4' - \frac{\varphi_0}{2d} (1+\lambda_4)] \right\} \\ &+ 2\varphi_0 \left[ \frac{k_1}{a}\, \lambda_1\, S_1\, S_1' - \frac{\Delta k}{b}\, S_2\, S_2' + \frac{k-k_1}{c}\, \lambda_3\, S_3\, S_3' - \frac{1-k}{d}\, S_4\, S_4' \right]. \end{aligned} \tag{A.51}$$

Here

$$g_{ab} = \frac{1}{a} + \frac{1}{b}\,, \qquad g_{bc} = \frac{1}{b} + \frac{1}{c}\,, \qquad g_{cd} = \frac{1}{c} + \frac{1}{d}\,, \qquad g_{ad} = \frac{1}{a} + \frac{1}{d}\,; \tag{A.52}$$

$$\lambda_1 = \exp\left[ -\frac{F k_1}{T(1-k)} - \frac{1-A_1}{T} \right], \qquad \lambda_2 = \exp\left[ \frac{F \Delta k}{T(1-k)} - \frac{\Delta A}{T} \right],$$

$$
\begin{aligned}
&\lambda_3 = \exp\left[\frac{F(k-k_2)}{T(1-k)} + \frac{A_2}{T}\right] , \qquad \lambda_4 = \exp\left(-\frac{1-F}{T}\right) , \\
&\lambda_5 = \exp\left[\frac{F(k-k_1)}{T(1-k)} + \frac{A_1}{T}\right] , \qquad \lambda_6 = \exp\left[\frac{F(1-k_1)}{T(1-k)} - \frac{1-A_1}{T}\right] , \\
&\lambda_7 = \exp\left[\frac{F(1-k_2)}{T(1-k)} - \frac{1-A_2}{T}\right] ;
\end{aligned}
\tag{A.53}
$$

$$
\begin{aligned}
S_1 &= -g_{ab} + \frac{g_{bc}}{\lambda_2} - \frac{g_{cd}}{\lambda_5} + \frac{g_{ad}}{\lambda_6} , \\
S_1' &= \frac{g_{ab}}{\lambda_6} - \frac{g_{bc}}{\lambda_7} + \frac{g_{cd}}{\lambda_4} - g_{ad} , \\
S_2 &= -g_{ab}\,(1-\varphi_0) + \frac{g_{bc}}{\lambda_2} - \frac{g_{cd}}{\lambda_5} + \frac{g_{ad}}{\lambda_6} , \\
S_2' &= g_{ab} - g_{bc}\,\lambda_2\,(1-\varphi_0) + g_{cd}\,\lambda_5\,(1-\varphi_0) - g_{ad}\,\lambda_6\,(1-\varphi_0) , \\
S_3 &= -g_{ab}\lambda_2(1-\varphi_0) + g_{bc}(1-\varphi_0) - \frac{g_{cd}}{\lambda_3} + \frac{g_{ad}}{\lambda_7} , \\
S_3' &= \frac{g_{ab}}{\lambda_5} - \frac{g_{bc}}{\lambda_3} + g_{cd}\,(1-\varphi_0) - g_{ad}\,\lambda_4\,(1-\varphi_0) , \\
S_4 &= -g_{ab}\,\lambda_5\,(1-\varphi_0) + g_{bc}\,\lambda_3\,(1-\varphi_0) - g_{cd}\,(1-\varphi_0) + \frac{g_{ad}}{\lambda_4} , \\
S_4' &= \frac{g_{ab}}{\lambda_5} - \frac{g_{bc}}{\lambda_3} + g_{cd} - g_{ad}\,\lambda_4\,(1-\varphi_0) .
\end{aligned}
\tag{A.54}
$$

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# List of publications

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2. E. Heinsalu, R. Tammelo, T. Örd, *Correlation between diffusion and coherence in the Brownian motion on tilted periodic potential*, Physica A (in press).

3. E. Heinsalu, T. Örd, R. Tammelo, *Diffusion and coherence in tilted piecewise linear double-periodic potentials* (submitted to Phys. Rev. E).

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