Transport in nonequilibrium systems with position-dependent mobility

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We propose a transport mechanism for overdamped diffusing particles. The mechanism is based on a position-dependent mobility and on breaking detailed balance. Using a two-state model, we show that the transport direction is given by the phase shift between mobility and potential or mobility and transition rate. No symmetry breaking potential as employed in ratchet-type transport models is needed.

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Transport of overdamped diffusing particles has been intensively studied in recent years [1–4]. These thermal ratchet models allow for a macroscopic directed motion of the diffusing particles without macroscopic external forces. Two key features of these models are that first the spatial symmetry of the system is broken by a periodic sawtooth potential (the ratchet) and second, the system is driven either by an external microscopic periodic forcing [1,3], by colored noise [5], or by considering a two-state system where the transition rates do not obey detailed balance [2]. Next to the physical applications of these models, it was also argued that they may be fundamental for the understanding of molecular motors.

A few years earlier Büttiker showed that state-dependent diffusion can induce transport [6]. This system is defined by an overdamped particle in a periodic symmetric potential with a periodic position-dependent diffusion rate. The spatial symmetry is broken by a phase shift between the potential and the diffusion rate, resulting in a probability current in equilibrium. The diffusion rate is related to the mobility μ and the temperature T by the Einstein relation $D=\mu k_B T$. Since the mobility is kept constant in this model, the diffusion rate varies due to a position-dependent temperature and the model actually focuses on transport in a periodic temperature field. However, the diffusion rate can vary due to position-dependent mobility, even for an isothermal process. The mobility of a spherical particle in a liquid is given by the Stokes law $\mu_0=(6\pi\eta a)^{-1}$ with η the viscosity of the liquid and a the radius of the particle. It is well known that this mobility becomes smaller when the particle approaches a wall surrounding the liquid [7,8]. A particle diffusing close to a surface has a position-dependent mobility and therefore also a position-dependent diffusion rate, although the temperature is constant.

To stress the difference between mobility and temperature, we set up the same model as Büttiker [6], however, the diffusion rate is position-dependent due to the mobility and not the temperature. Consider an overdamped diffusing particle in a periodic potential $V(x+L)=V(x)$ with $D(x)=\mu(x)k_B T$, $\mu(x+L)=\mu(x)$ and $T=$const. The Fokker-Planck equation for this system is given by

$$\partial_t P+\partial_x J=0, \tag{1}$$

with the probability current [8,9]

$$J=-\mu(x)(P\partial_x V+k_B T\partial_x P). \tag{2}$$

In the steady state, $\partial_t P=0$ and thus J is constant. Solving Eq. (2), the steady-state probability distribution is given by

$$P(x)=\left(C-\frac{J}{k_B T}\int^x \frac{\exp\left(\frac{V(x')}{k_B T}\right)}{\mu(x')}dx'\right)\exp\left(\frac{-V(x)}{k_B T}\right).$$

It follows that $P(x)\neq P(x+L)$ for nonvanishing J, since $\mu(x)$ is positive definite and the integral from x to $x+L$ does not vanish. A bounded equilibrium probability distribution is only possible for $J=0$, leading to the well-established result $P(x)=C\exp[-V(x)/k_B T]$ independent of the mobility. Hence a position-dependent mobility in this model does not lead to an equilibrium probability current contrary to a position-dependent temperature as was shown by Büttiker [6].

However, a position-dependent mobility does have an impact for systems out of equilibrium. Consider a one-dimensional system with the periodic mobility $\mu(x)=\mu_0[1+c\sin(2\pi x/L)]$ and without any potential. The amplitude of the modulation c is restricted to $0\leqslant c<1$. Particles diffuse freely until they are absorbed at one of the boundaries at $\pm L/2$. The probability for a particle initially released at $x=0$ to be absorbed at $L/2$ is [10]

$$p(L/2|0)=\int_{-L/2}^{0}\mu^{-1}(x)dx \Big/ \int_{-L/2}^{L/2}\mu^{-1}(x)dx$$

and $p(-L/2|0)=1-p(L/2|0)$. For $c=0.5$, the ratio of the probabilities can be calculated to $p(L/2|0)/p(-L/2|0)=2$. The particle is absorbed with higher probability at the boundary, where the mobility along the way is higher. Thus the mobility breaks the symmetry of this nonequilibrium problem. Note, however, that the integral mobility over a period L is the same in the positive and negative direction so that $p(L|0)/p(-L|0)=1$. On the other hand, the system would reach an equilibrium distribution that is constant and independent of the mobility with reflecting boundaries on both sides.

In order to take advantage of the mobility in a transport mechanism, the system needs to be driven out of equilibrium. Transport in a two-state model was studied by Prost

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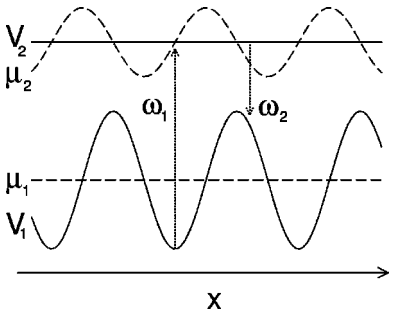

FIG. 1. The potential and mobility for the two-state model with symmetric potential. In state 1, the potential (solid line) is periodic, while the mobility (dashed line) is constant. In state 2, the potential (solid line) is constant, while the mobility (dashed line) is periodic. The transition rates between the states are ω_1 and ω_2. In order to obtain a net current, V_1 and μ_2 have to be phase shifted.

et al. [2]. They showed that transport can only occur when the transition rates between the states are driven away from their spontaneous values by an external action so that Boltzmann equilibrium is violated and when the spatial symmetry is broken by an asymmetric potential. Since symmetry can be broken by mobility, the question is whether transport in this model is possible with a symmetric potential together with a phase-shifted position-dependent mobility. The system is described by

$$\partial_t P_1 + \partial_x J_1 = -\omega_1 P_1 + \omega_2 P_2,$$

$$\partial_t P_2 + \partial_x J_2 = +\omega_1 P_1 - \omega_2 P_2, \tag{3}$$

with the probability currents

$$J_1 = -\mu_1(x)(P_1 \partial_x V_1 + k_B T \partial_x P_1),$$

$$J_2 = -\mu_2(x)(P_2 \partial_x V_2 + k_B T \partial_x P_2). \tag{4}$$

We assume a periodic symmetric potential at state 1 and a constant potential at state 2, while the mobility is constant at state 1 and a periodic function of the position at state 2: $V_1 = V_0 \cos(2\pi x/L)$, $V_2 = 0$, $\mu_1 = \mu_0$, $\mu_2 = \mu_0[1 + c \sin(2\pi x/L)]$. Detailed balance is violated by considering constant transition rates defined as $\omega_1 = \Omega \omega_2$, $\omega_2 = \text{const}$. The system is illustrated in Fig. 1.

A simple analytical solution of Eq. (3) is not possible under these conditions. We expand the probability densities in plane waves $P_l(x) = \Sigma_n a_l(n) \exp(i2\pi n x/L)$ with the state index $l = 1,2$. The resulting set of linear equations together with the norm condition

$$\int_{-L/2}^{L/2} P_1(x) + P_2(x) dx = 1 \tag{5}$$

can be solved using standard numerical methods [11]. Due to the smooth form of the potentials and mobilities the series expansion is well converged at $n = 40$. The resulting average transport velocity $v = (J_1 + J_2)L$ as a function of the dimensionless rate $L\sqrt{\omega_2/D_0}$ is shown in Fig. 2 (lines) for different values of the modulation amplitude c of μ_2. The typical stochastic-resonancelike behavior is found even quantitatively similar to the original model [2]. As expected, the

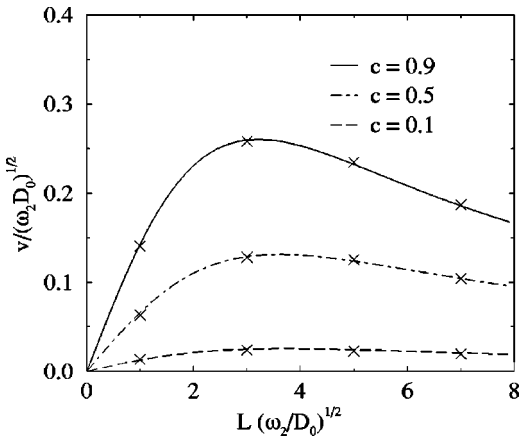

FIG. 2. The scaled drift velocity in the symmetric potential model for different values of the modulation amplitude c of the mobility μ_2. The lines are the direct solutions of the coupled Fokker-Planck equations, the crosses represent the results from the Monte Carlo simulation. The calculations are done for a particle with radius $a = 0.215$ μm in water, $L = 2a$, $T = 300$ K, $D_0 = \mu_0 k_B T$, $V_0 = -10 k_B T$ and $\Omega = 8$. The velocity is the average over 1000 particles after a simulation time of 5 s.

velocity decreases for decreasing c and vanishes for constant μ_2 given by $c = 0$ (not shown). Thus, the important role of the position-dependent mobility is clearly demonstrated.

As an alternative approach, we have investigated Eq. (3) by Monte Carlo simulations. The particle position at state l is updated according to [12,13]

$$\Delta x = [k_B T \partial_x \mu_l + \mu_l(-\partial_x V_l)]\Delta t + (2\Delta t \mu_l k_B T)^{1/2} X, \tag{6}$$

with X a normal distributed random number with zero mean and standard deviation equal to unity. Note the term proportional to the derivative of the mobility that is important for our model. The transition between the states are Poisson, that is, at each time step Δt, a particle in state 1 jumps to state 2, if $R < \omega_1 \Delta t$ with R a uniformly distributed random number between 0 and 1 and vice versa for a particle at state 2. The simulations (crosses) exhibit quantitative agreement with the direct solutions of Eq. (3) as can be seen in Fig. 2.

In this model, the direction of the probability current is defined by the phase shift between V_1 and μ_2. The mechanism can be understood in the following way (Fig. 1): A particle at state 1 drifts to the potential minimum. Undergoing a transition from the potential minimum at state 1 into state 2, the particle will experience a higher mobility on the right side in this state. Thus, the probability that the particle falls into the next potential well on the right side when returning to state 1 is higher than falling into the next well on the left side. The symmetry is broken and a net probability current to the right occurs. As it is typical for these two-state models transition rates, diffusion and period length are strongly interconnected. For instance, the system is most efficient at $L\sqrt{\omega_2 D_0} = 3.2$ for $c = 0.9$.

The main result from this section is that the role of symmetry braking can be overtaken by the mobility. Since this is the main function of the potential in the model of Prost *et al.* [2], one might wonder whether a transport mechanism in a two-state model without potentials is possible. The simplest scheme consists of a periodic mobility in state 1 and a con-

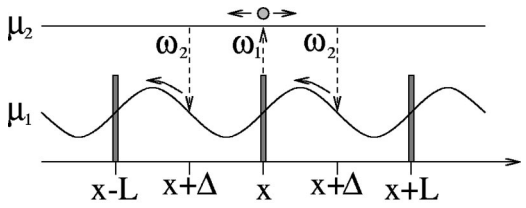

FIG. 3. Potential free two-state model. The mobility is periodic at state 1 and constant at state 2. The transition rate ω_1 is local while ω_2 is constant.

stant mobility in state 2 with constant potentials in both states: $\mu_1=\mu_0[1+c\sin(2\pi x/L)]$, $\mu_2=\mu_0$ and $V_1=V_2=0$. Detailed balance is broken by assuming a local transition rate $\omega_1=\Omega\theta(x)$ with the periodic function $\theta(x)=1$ for $|x-nL|<L/100$ and $\theta(x)=0$ otherwise (Fig. 3).

The local transition rate ω_1 is not suited for an expansion in plane waves and our approach for a direct solution of Eq. (3) fails. Therefore we report only results from numerical simulation where the treatment of local transition rates is trivial. As shown in Fig. 4, transport is obviously possible in the potential-free model. The average velocity shows qualitatively the same behavior as in Fig. 2; the transport velocity vanishes for $L\sqrt{\omega_2/D_0}\to 0$ and $L\sqrt{\omega_2/D_0}\to\infty$ and reaches one maximal value in between. However, the direction of the probability current is opposite. As shown in Fig. 3, a particle can make a transition from state 1 to state 2 at x. In state 2, the mobility is constant and the particle will with equal probability return to state 1 at $x+\Delta$ and $x-\Delta$. Back in state 1, the mobility is in both cases higher on the left side. The particle at $x+\Delta$ will with higher probability make the next transition to state 2 at x than at $x+L$. Similar, a particle at $x-\Delta$ will with higher probability make a transition to state 2 at $x-L$ than at x. There is a net drift toward the left side, resulting in a negative probability current.

The spatial symmetry is broken in this model by a phase shift of the mobility and the local transition rate of $L/4$ at state 1. If the transition rate ω_1 is localized at the maxima or minima of $\mu_1(x)$, one would expect no resulting probability current due to the symmetry of the system. We define the

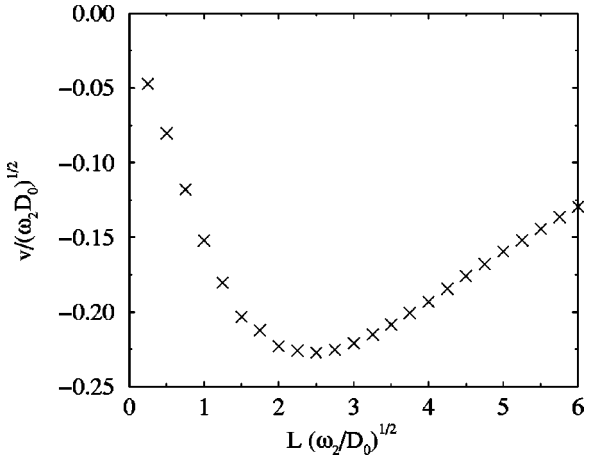

FIG. 4. The scaled drift velocity for the potential free model. The parameters are $c=0.9,\Omega=1000$. Other parameters are the same as in Fig. 2. The average of 5000 particles after a simulation time of 15 s is taken to obtain good statistics.

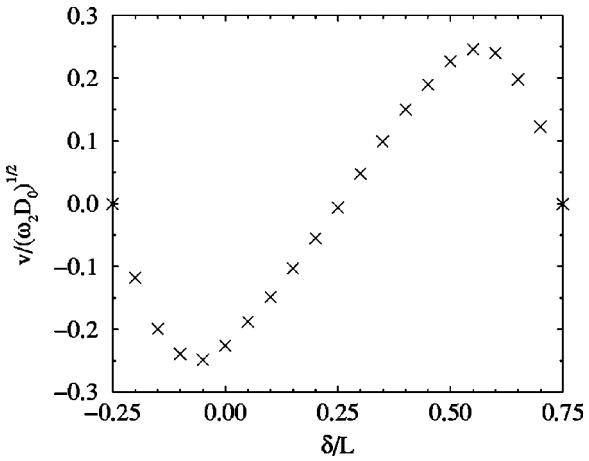

FIG. 5. Average velocity in the two-state model without potentials as a function of the phase-shift δ/L between the mobility μ_1 and the local transition rate ω_1.

phase shift δ by $\omega_1(x)=\Omega\theta(x-\delta)$. The transport velocity as a function of δ/L is shown in Fig. 5. For these simulations, ω_2 is set to the optimal value while all the other parameters remain the same. The velocity vanishes for $\delta/L=\pm 0.25$ and is positive for $\delta/L>0.25$. Depending on δ, the probability current becomes positive, negative, or vanishes. The extremal values for the average velocity are slightly shifted from $\delta=0$ and $\delta=0.5$.

To summarize, the simplest mobility-induced transport mechanism is an overdamped diffusing particle in a two-state model with (i) a periodic position-dependent mobility at one state and (ii) a local phase-shifted transition rate at the same state while mobility and transition rate in the other state are constant. The direction of the transport current depends on the phase shift between transition rate and mobility. Contrary to previous models, no macroscopic or microscopic forces are involved in the transport mechanism. The origin of the transport is a nonequilibrium statistical mechanics process.

A particle restricted to a one-dimensional diffusion in short distance to a rippled surface experiences a position-dependent mobility, since depending on its location it is closer to or further away from the surface. The molecular motor protein kinesin moves close along the periodic structure of the microtubule and will therefore experience a position-dependent mobility. The two-state model was proposed to be a model for molecular motors [2] and it was natural to investigate the role of a position-dependent mobility in this framework. We have shown that a position-dependent mobility can replace the ratchet potential, while the qualitative behavior of the motor remains the same. Thus the main role of the mobility in molecular motors might be in establishing a mechanism for breaking the spatial symmetry. Remarkably, members of the kinesin superfamily can move in different directions, although a given motor only moves in one direction [14]. The direction is shown to be a function of the motor domain that is very similar for all the members. In our model, the transport direction solely depends on the phase shift δ between either the local transition and the mobility or the mobility and the symmetric potential. Motors moving in different directions are distinguished by a different phase shift δ. Details of the role of a position-dependent

mobility in kinesin models will be discussed elsewhere [15].

In conclusion, we have shown that a position-dependent mobility can lead to transport very similar to that for models based on asymmetric potentials. Mobility can take over the role of the potential. However, the underlying mechanism is different: A particle with a position-dependent mobility tends to diffuse toward the higher mobility but is not forced to do so. Mobility-induced transport as a concept of possibilities rather than forces might be a fruitful way to think about biological, social, and financial systems that are so often out of equilibrium.

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