Rectification by hopping motion through nonsymmetric potentials: Local versus global bias

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(Received 28 February 2001; published 26 July 2001)

The hopping motion of noninteracting classical particles through nonsymmetric potentials is investigated in the case of alternating local bias. Different to the case of alternating global bias, a resonancelike behavior is observed. The system exhibits rectification effects in the regime of small to medium bias, whereas rectification effects are absent in the strong bias regime. Possible generalizations and applications are outlined.

DOI: 10.1103/PhysRevE.64.021109 PACS number(s): 05.60.Cd, 05.40.−a, 87.16.Nn

The question of how to achieve controlled directed motion on the mesoscale to nanoscale is of crucial importance for many fields of science, both from point of view of fundamental research as well as concerning possible future application to nanoscale machinery. Much of the research in this area has focused on the motion of particles in potentials without spatial symmetry under the influence of stochastic forces [1–12]. Here, one primarily attempts to understand under which conditions unidirectional motion of the particles in these so-called ratchet systems can occur, which connects the problem to the second law of thermodynamics [13] and to general symmetry considerations [14]. Second, the possible applicability to biological motors has been intensively discussed [15–18]. Most studies of ratchet systems are based on continuous diffusion models that are usually defined in terms of Langevin-type equations of motion, with a few exceptions focusing on hopping models [19–22]. Such hopping models, however, provide not only an intuitive physical picture of particles stochastically moving between sites relevant for microscopic transport processes [23] but also they are, generally speaking, just Markov processes, and may in that sense be expected to be more general and of broader applicability than Langevin-type descriptions.

In this paper, the hopping motion of noninteracting classical particles through nonsymmetric potentials is investigated in the case of alternating *local* bias. Different to the case of alternating *global* bias investigated previously [19–22], a resonancelike behavior as a function of bias strength is observed. The system exhibits rectification effects in the regime of small to medium bias, whereas rectification effects are absent in the strong bias regime. The motivation to study specifically the effects of a local modification of a nonsymmetric potential on the transport properties of an embedded particle origins in the fact that such a local alternation in the direct vicinity of the particle may provide a framework to construct active motor particles. This point and the important question of possible physical realizations are addressed in more detail at the end of this paper.

The specific topology under consideration is sketched in Fig. 1(a). The system consists of sites arranged along a chain, such that the site energies E_i are periodic with periodicity $\ell=4$ but do not exhibit inversion symmetry. The site energy E_i of site i is given by $E_i=(i \bmod 4)\epsilon$ with the energy difference $\epsilon>0$ being a parameter. Hence, one has $E_0=0$, $E_1=\epsilon$, $E_2=2\epsilon$, $E_3=3\epsilon$, $E_4=0$, $E_5=\epsilon$, and so on. The transition rates $\Gamma_{i\to i\pm1}$ from site i to the neighboring sites $i\pm1$ are given by $\Gamma_{i\to i\pm1}=\min\{1,\exp[-(E_{i\pm1}-E_i)/(k_B T)]\}$, where k_B denotes Boltzmann's constant and T the absolute temperature. As detailed balance is hence fulfilled, and as the system is homogenous on large length scales, no directed transport is observed in thermal equilibrium. However, when an alternating bias $b=\exp(\kappa/2)$ is applied along the chain, such that all left transition rates $\Gamma_{i\to i-1}$ are replaced by $\Gamma_{i\to i-1}b^{-1}$ and all right transition rates $\Gamma_{i\to i+1}$ by $\Gamma_{i\to i+1}b$, the system has been shown to exhibit rectification properties, where the net flux monotonously increases with increasing bias amplitude $|\kappa|$ [20].

Here, an alternative approach is proposed, which is different in principle to the *global* bias mentioned above: Instead of applying a bias that is equal for each site, an additional potential $\pi_i^{(t)}$ providing a *local* bias is added to the system, such that the spatially averaged bias is zero at any time. This additional potential shall depend on the site number i and on time by the number of steps t. The following discussion will focus on a specific simple form of $\pi_i^{(t)}$, which is defined as $\pi_i^{(t)}=\tau_t\sigma_i\delta$. Here, the parameter $\delta\geqslant0$ defines the strength of the bias. The two further quantities $\sigma_i=\pm1$ and $\tau_t=\pm1$ are responsible for the spatial and temporal dependence,

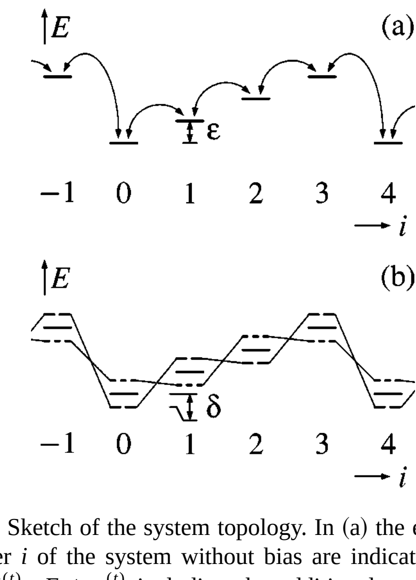

FIG. 1. Sketch of the system topology. In (a) the energies E_i vs site number i of the system without bias are indicated. In (b) the energies $E_i^{(t)}=E_i+\pi_i^{(t)}$ including the additional potential $\pi_i^{(t)}$ of strength δ are shown. As an example $\delta=3\epsilon/5$ is used. The two alternating realizations of the local bias are indicated by two different dashed lines, $\tau_t=1$ (dashed) and $\tau_t=-1$ (long dashed).

where $\sigma_i = 1-2(i \bmod 2) = \pm 1$ provides the spatial and $\tau_t = 1-2(t \bmod 2) = \pm 1$ yields the temporal dependence. Hence, the chosen additional potential $\pi_i^{(t)}$ is both alternating and periodic with period 2 in space and in time, $\pi_i^{(t)} = -\pi_{i\pm 1}^{(t)}$ and $\pi_i^{(t)} = -\pi_i^{(t\pm 1)}$. Furthermore, both spatial and temporal inversion symmetry is fulfilled, $\pi_i^{(t)} = \pi_{-i}^{(t)}$ and $\pi_i^{(t)} = \pi_i^{(-t)}$. Adding this additional potential to the constant site energies E_i yields time dependent site energies $E_i^{(t)} = E_i + \pi_i^{(t)}$, see Fig. 1(b). The resulting time dependent transition rates are given by $\Gamma_{i\to i\pm 1}^{(t)} = \min\{1, \exp[-(E_{i\pm 1}^{(t)} - E_i^{(t)})/(k_B T)]\}$.

It is worthwhile to mention that this approach of a local modification of the site energies is to some extend motivated by a recent study of a particular ratchet system, where within a continuous diffusion model the motion of a particle subject to a two-wave potential has been investigated [24]. The two-wave potential is composed of a spatially nonsymmetric ratchet potential and a spatially symmetric potential of equal strength and periodicity, where the latter is translated with respect to the first, either in an oscillatory manner or randomly. As a result of the relative translation, a quite efficient directed transport of the embedded particle has been observed (for a simple physical realization of this ratchet system based entirely on the Coulomb interaction see Ref. [25]). Comparing this continuous diffusion model with the current hopping model, it should be noted that the local bias' time evolution $\pi_i^{(t)} \to \pi_i^{(t+1)}$ is equivalent to a lateral translation $\pi_i^{(t)} \to \pi_{i\pm 1}^{(t)}$. This effective lateral translation of $\pi_i^{(t)}$ is, however, not performed in any specific direction, as generally $\pi_{i-1}^{(t)} = \pi_{i+1}^{(t)}$.

When comparing this hopping system with the ones studied earlier [19–22], it is important to stress that the alternation of the local bias is done with the frequency of the individual particle hops. Hence, different to the related previous study of rectification of a global bias [20], the system is investigated in the high frequency regime, and thus a discussion in the framework of stationary solutions is not possible. Therefore, an analytical treatment seems not to be feasible, and the further discussion will rely on a numerical investigation of the system [26].

During the numerical simulation, the mean displacement of a tracer particle in the systems in units of number of sites, $\overline{\Delta i}$, after a large number of time steps $N = 10^6$ is obtained. The mean velocity $\overline{v}$ is then defined as $\overline{v} = \overline{\Delta i}/N$, in units of gained number of sites per time step. The numerically obtained result for $\overline{v}$ vs local bias strength δ for several values of energy difference ϵ is shown in Fig. 2. In the current system rectification effects are governed by the interplay of the two energy scales ϵ and δ, and hence a resonancelike behavior is observed. The respective maximum $\overline{v}$ in the mean velocity is found when $\delta = \delta_{\max} = \epsilon/2$ for given ϵ. This can be intuitively understood by noting that for $2\delta = \epsilon$ the neighboring sites of the energy "stairs" are timewise on the same energy value. Therefore, the motion to the right side is particularly easy, whereas the motion to the left is hindered by the large energy gap, whose value alternates between $3\epsilon + 2\delta_{\max} = 4\epsilon$ and $3\epsilon - 2\delta_{\max} = 2\epsilon$. For even larger values of δ, the mean velocity $\overline{v}$ and hence the efficiency of the directed transport drops, and reaches finally zero as soon as the local bias reaches the value $\delta = \delta_{\text{end}} = 3\epsilon/2$ for given ϵ. In the case when $2\delta = 3\epsilon$, the alternating potential is equal to the large energy gaps in the original system, and hence these gaps hindering the motion to the left are timewise erased. As a result, the ratchet character of the total potential vanishes, and the motion gets purely diffusive.

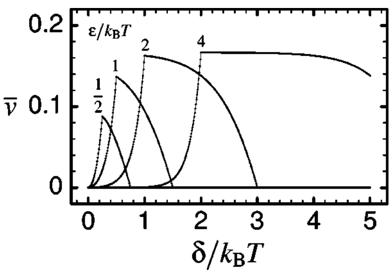

FIG. 2. Plot of the mean velocity $\overline{v}$ vs local bias strength δ for different values of the energy difference $\epsilon/(k_B T) = 1/2$, $\epsilon/(k_B T) = 1$, $\epsilon/(k_B T) = 2$, and $\epsilon/(k_B T) = 4$ (from left to right). The results are obtained by averaging over 100 configurations of 10^6 time steps each.

Although the obtained curves are apparently similar and one might intuitively expect scaling behavior with the ratio δ/ϵ, it should be stressed that no exact scaling of the curves in Fig. 2 is possible. The reason for the counterintuitive absence of scaling is that the dynamics of the system is governed not only by the two competing energy scales δ and ϵ, and their ratio δ/ϵ. Additionally, there are two competing time scales in the system, the time scale 1 given by the time between the alternation of the local bias, and the time scale $\exp[\epsilon/(k_B T)]$ given by the mean number of tries before an uphill jump is done.

Several simple generalization within the picture of local bias are possible. So far the applied local bias exhibits periodicity both in space and in time. Alternatively, one may define the quantity $\tau_t = \pm 1$ providing the temporal dependence to be a random variable, keeping the spatial periodicity only. In the case of τ_t being randomly chosen in every time step, the obtained mean velocity $\overline{v}$ in units of gained number of sites per time step vs local bias strength δ for several values of energy difference ϵ is shown in Fig. 3. As before, a resonancelike behavior is observed. The maximum $\overline{v}_{\max}$ in the mean velocity is, however, observed for larger values of δ with $\delta_{\max} \approx \epsilon$ for given ϵ. Additionally, the resonance is much broader than before, and the system is hence less sensitive to the right choice of the local bias strength to achieve an efficient particle transport. Besides the position $\delta_{\max}$ of the curve's maximum, one observes two further distinguished values of δ for each ϵ, $\delta_1 = \epsilon/2$, and $\delta_2 = 3\epsilon/2$, where the curves are not differentiable. These two distinguished values of δ are the reminiscence of the two respective values $\delta_{\max}$ and δ_{end} observed in the data shown in Fig. 2. Analogously to the case of periodic τ_t discussed above, the curves are apparently similar, but they do not again exhibit scaling behavior. As it is obvious when comparing Figs. 2 and 3, a temporal periodicity is found to be helpful to

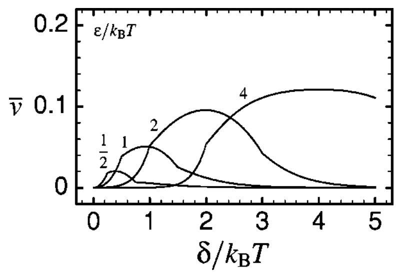

FIG. 3. Plot of the mean velocity $\overline{v}$ vs local bias strength δ for different values of the energy difference $\epsilon/(k_B T)=1/2$, $\epsilon/(k_B T)=1$, $\epsilon/(k_B T)=2$, and $\epsilon/(k_B T)=4$ (from left to right) for the case of randomly chosen τ_t. The results are obtained by averaging over 100 configurations of 10^6 time steps each.

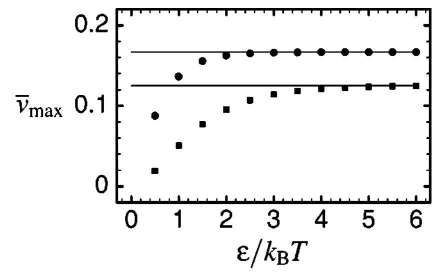

FIG. 4. Plot of the maximum mean velocity $\overline{v}_{\max}$ vs the energy difference ϵ for $\tau_t = 1-2(t \bmod 2)$ (circles) and randomly chosen τ_t (squares). In the first case $\delta=\epsilon/2$ is used, whereas in the second case the result is for $\delta=\epsilon$. The horizontal lines indicate the values 1/6 and 1/8. The results are obtained by averaging over 100 configurations of 10^6 timesteps each.

achieve an efficient transport, as the maximum mean velocity $\overline{v}_{\max}$ is generally larger with periodicity in time than without, but it is not a necessary condition. The somewhat smaller maximum mean velocity $\overline{v}_{\max}$ is, however, counterbalanced by a much broader interval for values of δ for which an almost maximum performance is observed.

When focusing on the influence of the energy difference ϵ on the maximum value $\overline{v}_{\max}$ of the mean velocity, one finds a strong increase for small values of ϵ, and a saturation for large values of ϵ, see Fig. 4. The saturation value $\overline{v}_{\max} \to 0.1667$ (i.e., $\cong 1/6$) is reached for $\epsilon/(k_B T) \gtrsim 3$ in the case of periodic τ_t, whereas in the case of randomly chosen τ_t the saturation value $\overline{v}_{\max} \to 0.125$ (i.e., $\cong 1/8$) is reached for $\epsilon/(k_B T) \gtrsim 6$. It should be noted that this saturation value decreases with increasing periodicity ℓ of the underlying nonsymmetric potential. In case of a system with periodicity $\ell=6$ instead of 4 [i.e., when $E_i=(i \bmod 6)\epsilon$], one finds $\overline{v}_{\max} \to 0.125$ (i.e., $\cong 1/8$) for periodic τ_t and $\overline{v}_{\max} \to 0.0833$ (i.e., $\cong 1/12$) for randomly chosen τ_t. Analogously, for the periodicity $\ell=8$ [i.e., when $E_i=(i \mod 8)\epsilon$], one obtains $\overline{v}_{\max} \to 0.1$ (i.e., $\cong 1/10$), and $\overline{v}_{\max} \to 0.0625$ (i.e., $\cong 1/16$), respectively. Therefore, one finds the saturation value to decrease as a function of the periodicity $\ell \in \{4,6,8\}$ as $\cong 1/(\ell+2)$ in the case of periodic τ_t, whereas in the case of randomly chosen τ_t one observes a decrease as $\cong 1/(2\ell)$.

Putting the above results in the context of a simple physical realization, one might think of a particle having a two-value internal degree of freedom such as a spin. This particle hops through a nonsymmetric potential, where the site energies are assumed to be slightly altered depending on the particle's internal degree of freedom. The alternation is in such a way that for the first (second) value of the internal degree of freedom, a given site energy is lowered (raised) by a certain amount of energy, the next site is raised (lowered) in energy, the next site, but one, is lowered (raised) again, and so on. In case it is possible to change the particle's internal degree of freedom supplying energy to the system, even if this is done in a random fashion, the particle will perform an efficient directed motion through the potential.

In summary, it has been shown that an alternating local bias added to a system containing a nonsymmetric potential leads to a quite efficient directed transport of an embedded particle. Coming back to the original question of controlled direction motion on the mesoscale to nanoscale, it should be stressed that such a *local* modification of the potential in the direct vicinity of the particle subject to it (or a modification of the embedding potential by a *local* alternation inside the particle having an internal structure as in Ref. [25]) corresponds closer to the framework of an *active* motor particle, whereas a *global* bias fits better into the framework of a *passively* pumped particle. This active character, however, can be expected to be of importance for possible applicability of this and other concepts to nanoscale machinery.

Helpful comments on the manuscript by A. Ordemann are gratefully acknowledged.

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[26] During the numerical simulations, for each single configuration a particle is placed onto the chain at site 0. Then, in each diffusion step t, at first one of the two available nearest neighbors $j=i\pm 1$ of the current site i is chosen randomly with equal probability. Second, the jump is either performed with probability $\Gamma^{(t)}_{i\rightarrow j}$, whereas with probability $1-\Gamma^{(t)}_{i\rightarrow j}$ the particle remains at site i. After 10^6 time steps, the displacement Δi is obtained. The whole simulation is repeated, and the mean displacement $\overline{\Delta i}$ is calculated by averaging over 100 independent configurations.