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Driven lattice gas as a ratchet and pawl machine

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Boundary-induced transport in particle systems with anomalous diffusion exhibits rectification, negative resistance, and hysteresis phenomena depending on the way the drive acts on the boundary. The solvable case of a one-dimensional (1D) system characterized by a power-law diffusion coefficient and coupled to two particle reservoirs at different chemical potential is examined. In particular, it is shown that a microscopic realization of such a diffusion model is provided by a 3D driven lattice gas with kinetic constraints, in which energy barriers are absent and the local microscopic reversibility holds.

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I. INTRODUCTION

Macroscopic motion generally results from the action of nonzero macroscopic forces. Ratchets are systems which are able to develop a directed motion in the absence of macroscopic forces. Since the early days of kinetic theory, devices of this sort have been used as a means to probe the statistical nature of the second law [1]. A celebrated example is the Smoluchowski-Feynman ratchet and pawl machine [2,3]. In the last decade, the interest in ratchet systems has been mainly motivated by motor proteins and new separation techniques [4]. According to the Curie principle, a directed transport may arise even in the absence of a macroscopic bias provided that both parity and time-reversal symmetry are broken. Closely related is the nonmonotonic behavior of the particle current in response to a driving force, known as negative incremental resistance (NR). Nonlinear transport properties are a crucial ingredient in the complex behavior of many biological and artificial systems. Typical NR rectifying devices are the tunnel diode and the sodium channel. There is interest in understanding the microscopic origin of such a behavior (which in a tunnel diode is quantum mechanical) and to provide classic (stochastic or deterministic) analogs [5,6]. Cecchi and Magnasco have suggested a purely geometric mechanism in which the time scales involved in the particle motion do not follow the Arrhenius-Kramers law but rather depend on the existence of purely ‘‘entropic’’ barriers [6].

In this article we show that similar nonlinear transport phenomena may occur in a kinetic lattice-gas model in which there are no energetic barriers and no local breaking of the detailed balance (time-reversal symmetry). We first consider transport properties in a one-dimensional (1D) solvable model of a boundary-driven system with a power-law vanishing diffusion coefficient. The anomalous diffusion coefficient induces a nonlinear relation between the particle current and boundary densities, which in turn is responsible for rectification and negative resistance. For the particular case we consider here these features can be analytically investigated. We then show that a microscopic realization of such a restricted diffusion model is provided by a 3D boundary-driven lattice gas with reversible kinetic constraints, which is coupled to two particle reservoirs.

II. THE DIFFUSION MODEL

Consider a transport process in a slab of size $2L$ which is described by the one-dimensional diffusion equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial z}\left[D_{\phi}(\rho)\,\frac{\partial \rho}{\partial z}\right], \tag{1}$$

where $\rho(z,t)$ is the local particle density, and $|z|\leqslant L$. The diffusion coefficient $D_{\phi}(\rho)$ vanishes at a critical threshold density, ρ_c, as a power law with an exponent $\phi \geqslant 0$:

$$D_{\phi}(\rho) = D_0(1+\phi)(\rho_c-\rho)^{\phi}. \tag{2}$$

The system boundaries, located at $z=\pm L$, are in diffusive contact with two-particle reservoirs at chemical potential $\mu_{\pm}$, which keep the boundary densities at

$$\rho(\pm L,t) = \rho_{\pm}, \quad \forall \quad t \geqslant 0. \tag{3}$$

When $\rho_+ = \rho_- < \rho_c$, the characteristic relaxation time is finite and the system attains an equilibrium state characterized by a flat profile. When $\rho_{\pm} = \rho_c$, the system approaches the critical density by a power law and the breaking of time-translation invariance ensues [9]. The model was indeed introduced in Ref. [9] with the purpose of understanding aging in a kinetically constrained lattice-gas [7,8]. Here we consider the nonequilibrium stationary properties of a system with $\rho_+ \neq \rho_-$ and ρ_+, $\rho_- < \rho_c$. In this case the relaxation time is still finite for any finite L, and the steady-state density profile, $\rho(z)$, is easily computed:

$$\rho_c - \rho(z) = (La_+ - za_-)^{1/(1+\phi)}, \tag{4}$$

where the constants $a_{\pm}$ are determined by the boundary condition (3),

$$a_{\pm} = \frac{1}{2L}\left[(\rho_c-\rho_-)^{l+\phi} \pm (\rho_c-\rho_+)^{1+\phi}\right]. \tag{5}$$

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The particle current is then obtained as $J=D(\rho)\partial_z\rho$, which gives

$$J(\rho_-,\rho_-)=\frac{D_0}{2L}[(\rho_c-\rho_-)^{1+\phi}-(\rho_c-\rho_+)^{1+\phi}]. \quad (6)$$

The expression of the current has two interesting features: it is nonlinear and does not depend only on the single variable $\Delta\rho=\rho_+-\rho_-$. In the limit $\rho_\pm \ll \rho_c$ the density profile is linear, and the Fick's law $J\sim\Delta\rho$ is recovered in agreement with the linear-response theory. At high enough density, however, this is not the case and more interesting transport phenomena emerge. In the following we explore the implication of Eq. (6) in the nonlinear regime for some relevant cases.

A. Rectification

To begin with we consider, as in [10], a boundary potential $\Delta\rho(t)=\rho_+(t)-\rho_-(t)$ which is a periodic asymmetric step function of time with zero average over the period τ:

$$\Delta\rho(t)=\begin{cases} 1-\tau_0/\tau, & t\in[0,\tau_0]; \\ -\tau_0/\tau, & t\in[\tau_0,\tau]. \end{cases} \quad (7)$$

The average current over the period is

$$J_{\mathrm{av}}=\frac{1}{\tau}\int_0^\tau J(\rho_+(t),\rho_-(t))dt. \quad (8)$$

In Fig. 1 we show a plot of J_{av} vs the asymmetry parameter $\alpha=\tau/\tau_0-1$, for the case in which $\rho_-(t)=0$ for $t\in[0,\tau_0]$, and $\rho_+(t)=0$ for $t\in[\tau_0,\tau]$. For $\alpha=1$ the potential is symmetric, $\Delta\rho(\tau_0+t)=-\Delta\rho(t)$, and no net average current can flow through the system; the rectification effect, i.e., a nonzero average net current, occurs for any $\alpha\neq1$. As in other ratchet systems, there is a certain value of α for which an optimal pumping condition exists. The current direction is determined only by α; for $\alpha>1$ the current is negative such that $J_{\mathrm{av}}(\alpha)=-J_{\mathrm{av}}(1/\alpha)$. However, if the density of one boundary, say $\rho_-(\rho_+)$, is kept fixed to a nonzero value, there is no current inversion; J_{av} is always negative (positive) regardless of the value of the asymmetry, α, see Fig. 1(b). In this case, the net current is nonzero even for a symmetric potential $\Delta\rho(t)$, provided only the diffusion is not normal, $\phi\neq0$. This is not in contradiction with the Curie principle, as parity is explicitly broken; $\rho(-L,t)\neq\rho(L,t)$, while the boundary dissipation breaks the time-reversal symmetry. More generally, one may also consider a symmetric potential that changes adiabatically according to suitable paths in the space of variables (ρ_+,ρ_-), and finds similar rectification properties.

B. Negative resistance and hysteresis

To further explore the nonlinear transport regime we looked for situations in which an increasing driving force leads to a decreasing particle current. To keep things simple, we consider the case in which the ratio of the boundary densities, $\delta=\rho_-/\rho_+$, is fixed, and study the stationary point of

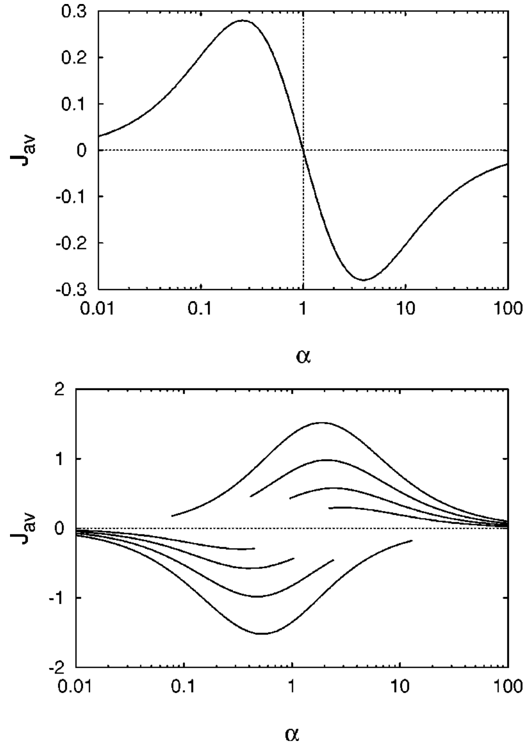

FIG. 1. Rectification. Average current J_{av} plotted against the asymmetry parameter $\alpha=\tau/\tau_0-1$ for a boundary periodic potential with zero average over the period $[0,\ \tau]$ (in both figures we set $\tau=1$). (a) $\rho_-(t)=0$ for $t\in[0,\tau_0]$, and $\rho_+(t)=0$ for $t\in[\tau_0,\tau]$. (b) The curves with $J_{\mathrm{av}}>0$ ($J_{\mathrm{av}}<0$) correspond to a fixed ρ_+ (ρ_-). In both cases there is a value of α for which an optimal pumping condition exists.

Eq. (6) at constant δ. This is done by the method of Lagrange multipliers, which gives the maximum of the current

$$J_{\max}=\frac{\rho_c^{1+\phi}}{1+\phi}\frac{(1-\delta)^{1+\phi}}{(1-\delta^{1/(1+\phi)})^{\phi}} \quad (9)$$

at

$$\frac{\rho_+^{\max}}{\rho_c}=\frac{1-\delta^{1/\phi}}{1-\delta^{(1+\phi)/\phi}},\quad \frac{\rho_-^{\max}}{\rho_c}=\delta\frac{1-\delta^{1/\phi}}{1-\delta^{(1+\phi)/\phi}}. \quad (10)$$

Increasing the driving force above this value leads to a decreasing particle current. The nonmonotonic behavior of the current is shown in Fig. 2 as a function of the drive $\Delta\rho=\rho_+-\rho_-$ for different δ. In the limit of small density gradient Fick's law is correctly recovered (the dotted line in Fig. 2). The higher the δ the smaller the range in which the linear relation holds. The negative resistance found here is a consequence of the fact that the current depends in a nonlinear way on both reservoir densities, which in our model follows specifically from a power-law vanishing diffusion coefficient. This last feature is commonly observed, e.g., in colloids and hard-sphere systems near their random close-packing limit. In the next section we shall see how, at microscopic level, negative resistance and rectification may occur in the absence of any energetic barriers to the particle

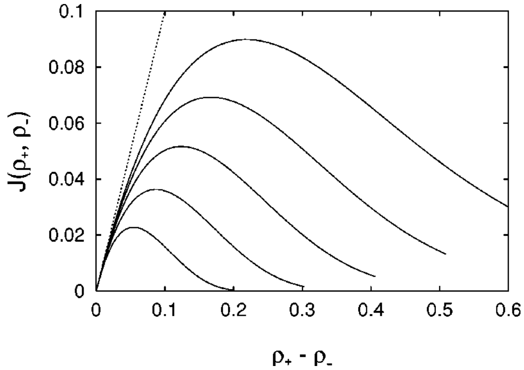

FIG. 2. Negative resistance. The particle current $J(\rho_+,\rho_-)$ is plotted versus the potential $\rho_+-\rho_-$ for different values of the ratio $\delta=\rho_-/\rho_+=0.4$, 0.5, 0.6, 0.7, and 0.8 (from top to bottom). The dotted line represents Fick's law, which is recovered in the limit of small density gradient.

motion, through a purely ''entropic'' mechanism as has been suggested in Ref. [6]. These phenomena are intimately associated with the possibility of having a hysteretic response. If we consider a loop in the plane (ρ_+,ρ_-) it can be shown that the particle current responds to the driving force by following a clockwise hysteresis cycle (see Fig. 3). Finally, we mention that similar nonlinear transport properties also appear in the presence of a divergent diffusion coefficient, $\phi<0$. The related diffusion equation was studied by Carlson and co-workers in an attempt to provide a continuum description of self-organizing critical systems [11].

C. The driven lattice gas

We now show that a microscopic realization of the above diffusion model does indeed exist. It is provided by a kinetically constrained lattice-gas, boundary driven in a nonequilibrium stationary state by a chemical-potential difference. The bulk dynamic of the model (defined on a cubic lattice) consists in moving a particle to a neighboring empty site if the particle has less than four nearest-neighboring particles before and after it has moved, consistent with detailed balance [7]. The boundary dynamic mimics the contact of the system with a particle reservoir at chemical potential $\mu_\pm$. It is simulated according to the usual Monte Carlo rule: if a randomly chosen site on the layer is empty, a new particle is added; otherwise, if the site is occupied, the particle is removed with probability $e^{-\mu_\pm}$ ($\mu_\pm\geqslant 0$, we set $k_BT=1$). The global effect of the reservoirs is to fix the boundary densities at two different values ρ_+ and ρ_-, driving a current through the system. The aging dynamics of the system when the two reservoirs are at the same chemical potential was first investigated in [8,9]. As the density gets closer to the threshold value $\rho_c\simeq 0.88$, the diffusion coefficient approaches zero as a power law, Eq. (2), with $\phi=3.1$ [7]. For our purposes it is sufficient to show that close to the threshold ρ_c and in the presence of two reservoirs, the system approaches a steady state characterized by a density profile which is exactly described by the Eq. (4). In Fig. 4 the density profile obtained in a Monte Carlo simulation is compared with the one predicted by the anomalous diffusion equation using the above values of ρ_c and ϕ. There is excellent agreement between the two. The small discrepancy observable near the higher density edge is a finite-size effect which tends to disappear as the thermodynamic limit $L\to\infty$ is approached. In Fig. 4 for comparison we show the numerical density profiles of both the usual boundary driven 3D lattice gas (obtained by removing the kinetic constraints) and that predicted by the normal diffusion equation. These results suggest that the nonlinear nature of the density profile, and consequently the nonlinear transport, is essentially determined by the presence of blocked configurations induced by the kinetic constraints.

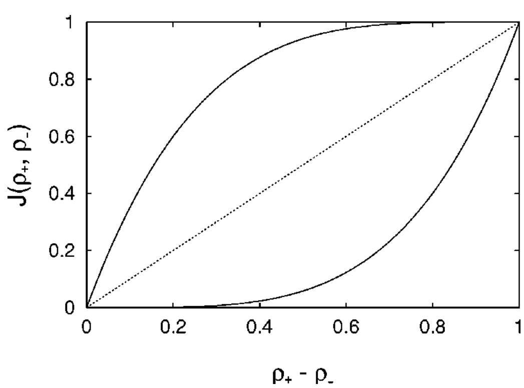

FIG. 3. Hysteresis. Response of the current J to a cyclic change of the potential $\Delta\rho=\rho_+-\rho_-$. The loop in the plane (ρ_+,ρ_-) is carried out in three steps: starting from $\rho_+=\rho_-=\rho_a$ the value of ρ_+ is increased up to ρ_b keeping constant $\rho_-=\rho_a$ (upper curve); then ρ_- is increased from ρ_a to ρ_b while ρ_+ is fixed to ρ_b (lower curve); finally ρ_+ and ρ_- are decreased to ρ_a keeping $\rho_+=\rho_-$. We set $\rho_a=0$ and $\rho_b=1$. The continuous line corresponds to the case $\rho_c=1$ and $\phi=3.1$ (anomalous diffusion), while the dashed straight line—absence of hysteresis—corresponds to normal diffusion ($\phi=0$).

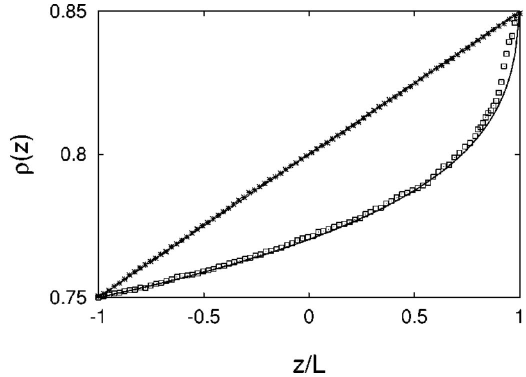

FIG. 4. Density profile in a boundary-driven lattice gas coupled to two-particle reservoir at density $\rho_+=\rho(L)=0.85$ and $\rho_-=\rho(-L)=0.75$ (squares), with $L=160$ and transverse surface 20^2. The continuous smooth line represents the analytic profile predicted by the diffusion equation, Eq. (4). Also shown, for comparison, is the linear profile corresponding to a normal diffusion coefficient (dashed line), and the numerical simulation data obtained by removing the kinetic constraints (stars).

III. SUMMARY AND CONCLUSION

In this article we have shown that an analytically solvable model of boundary-induced transport exhibits rectification, hysteresis, and negative resistance phenomena. We have also shown that such features may occur in driven lattice-gas models where local detailed balance holds and dissipation is only forced on the boundary. In particular, we have presented numerical results supporting the hypothesis that the diffusion model represents the hydrodynamic limit of a driven lattice gas with kinetic constraints. The efficiency of the system in the presence of an external load and the interplay of the boundary-driving force with a spatially varying potential, may also be of interest. Since there are no energetic barriers to the motion of particles this model provides another example of a ratchet system based on the mechanism of entropic trapping [6]. The relationship between the macroscopic diffusion model and the microscopic lattice gas sheds some light on the nonlinear nature of transport properties. On one hand, they are due to the nonlinear dependence of the density profile on both boundary densities, not simply on their difference. On the other hand, the nonlinear density profile in the driven lattice gas follows from the presence of blocked configurations. This suggests that the steady-state transport properties, like some features of aging systems, are essentially determined by an extensive entropy of blocked configurations. It is tempting to speculate that even in such cases the invariant dynamic measure could be defined in terms of a suitable generalization of the Edwards hypothesis [12].

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