Boundary-Induced Phase Transitions in Driven Diffusive Systems

Joachim Krug
IBM Research Division, T. J. Watson Research Center, Yorktown Heights, New York 10598
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Steady states of driven lattice gases with open boundaries are investigated. Particles are fed into the system at one edge, travel under the action of an external field, and leave the system at the opposite edge. Two types of phase transitions involving nonanalytic changes in the density profiles and the particle number fluctuation spectra are encountered upon varying the feeding rate and the particle interactions, and associated diverging length scales are identified. The principle governing the transitions is the tendency of the system to maximize the transported current.

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In the absence of spontaneously broken symmetries the bulk state of a system in thermal equilibrium is independent of the imposed boundary conditions. This need no longer be true if a nonequilibrium steady state is maintained through the action of external forces. The present paper explores the surprising richness of boundary-induced bulk effects that can occur in the particular case of driven diffusive systems, which have been widely studied as prototypes of nonequilibrium steady states [1-7]. Such systems are characterized by a locally conserved density, and a uniform external field which sets up a steady mass current. Roughly speaking, it is this current which transports information from the boundaries into the bulk of the system and thereby permits the boundary conditions in certain regimes to dominate the bulk [4,5]. I will demonstrate that the subtle interplay between boundary conditions and bulk transport can lead to behavior reminiscent of second- and first-order phase transitions even in one-dimensional systems with short-range interactions. In contrast to previous studies [1-5] which have concentrated on the nonequilibrium equivalent of the Ising phase transition, the transitions described here have no counterpart in equilibrium systems.

Microscopically, a driven diffusive system is modeled as a lattice gas [1]. Particles occupy the sites of a d-dimensional lattice with at most one particle per site. They jump stochastically to vacant nearest-neighbor sites according to rates which may depend on the local environment. The external field biases jump in the positive x direction. In a homogeneous state of density $\rho \in (0,1)$ the field maintains a steady current $j(\rho)$. For small densities $j \sim \rho$ while for $\rho \rightarrow 1$ the current vanishes due to mutual blocking of the particles. Hence in the simplest case the current has a single maximum j^* at some density ρ^*, $j^* = j(\rho^*)$.

Consider now a system of finite extension L in the x direction and infinite extension in the other $d-1$ directions. The boundaries are in contact with particle reservoirs [8] of density ρ_0 at $x=0$, and zero density at $x=L$, i.e., particles are injected at $x=0$ and leave the system at $x=L$. This induces a density gradient which is expected to generate an excess current j_{ex} in addition to the systematic current $j(\rho)$. Stationarity requires the total current to be constant everywhere, $j_{\mathrm{ex}} + j(\rho) \equiv J$. I claim that the total current is always maximized, in the sense that in the limit $L \rightarrow \infty$,

$$J = \max_{\rho \in [0,\rho_0]} j(\rho) . \tag{1}$$

To see this, we anticipate the general shape of the density profile, to be discussed in more detail below. The profile is monotonously decreasing, with a plateau at some density $\bar{\rho} \in [0,\rho_0]$ and appreciable density variations only in the boundary regions which occupy a vanishing fraction of the system for large L (see Fig. 1). Hence j_{ex} can be neglected in the bulk and $J = j(\bar{\rho})$. Suppose that $j(\rho') > j(\bar{\rho})$ for some $\rho' \in (0,\rho_0)$. The profile must pass through the value ρ' in one of the boundary regions where $j_{\mathrm{ex}} > 0$. The total current at this point therefore would exceed J. This violates stationarity, whence (1) is established. A numerical example of the predicted behavior is shown in Fig. 2. The simulations were carried out for a one-dimensional lattice gas with hard-core interactions [7] and jumps only in the positive x direction [9]. In this

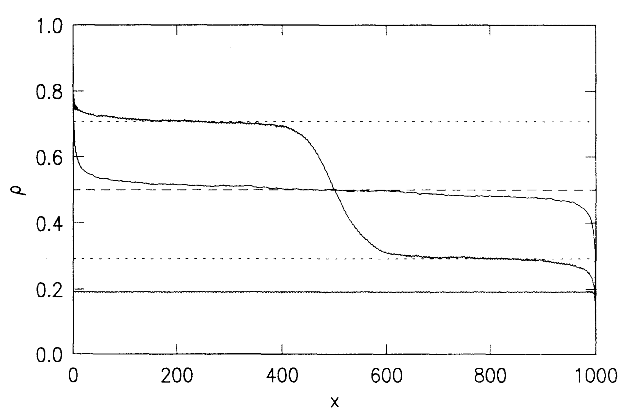

FIG. 1. Density profiles of one-dimensional driven lattice gases. The uniform profiles correspond to $\rho_0 = 1$, $\beta = 0$ (top) and $\rho_0 = 0.19$, $\beta = 1$ (bottom). The nonuniform profile corresponds to $\rho_0 = 0.8$, $\beta = \infty$. In each case the density was averaged over 10^6 attempted jumps per site. The dashed line is at $\rho = \frac{1}{2}$; the dotted lines indicate the predicted plateau densities $\rho_{1,2}$ at $\beta = \infty$.

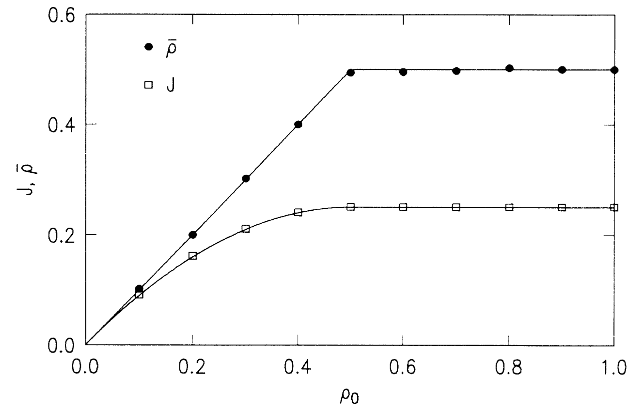

FIG. 2. Spatially averaged density $\bar{\rho}$ and current J as a function of the boundary density ρ_0 for the hard-core exclusion model ($\beta=0$). Each data point is an average over 125000 attempts per site and the system size is $L=1000$. The solid lines are the predictions of Eq. (1).

case $j(\rho)=\rho(1-\rho)$, so $j^*=\frac{1}{4}$ and $\rho^*=\frac{1}{2}$. Note that (1) implies a nonanalytic variation of J and $\bar{\rho}$ when ρ_0 passes through ρ^*. This constitutes the first type of phase transition found in these systems. We shall see below that the two "phases" $\rho_0>\rho^*$ and $\rho_0<\rho^*$ are qualitatively different, and that a diverging length scale can be associated with the transition.

The purpose of the previous discussion was to illustrate that the occurrence of a transition at $\rho_0=\rho^*$ is largely independent of the form of the excess current $j_{\rm ex}$. To proceed, we postulate a diffusive excess current, $j_{\rm ex}=-D\,\partial\rho/\partial x$. The stationarity condition then becomes an ordinary differential equation [5] from which the profile is readily computed,

$$D\frac{d\rho}{dx}=j(\rho)-J,\;\;\rho(0)=\rho_0,\;\;\rho(L)=0. \tag{2}$$

Note that the value of J is determined through the boundary conditions. In the limit $L\to\infty$ (1) is recovered. In the following I consider only the infinite system. For $\rho_0>\rho^*$ the density profile approaches the plateau at $\bar{\rho}=\rho^*$ as a power law [10], $\rho(x)-\rho^*\simeq(D/x)^{1/(n-1)}$, where n is the order of the maximum of $j(\rho)$, $j^*-j(\rho)\sim(\rho-\rho^*)^n$. In the generic case $n=2$ the profile decays as $1/x$. The asymptotic decay sets in beyond a crossover length scale ξ_c which is obtained by equating the power law to $\rho_0-\rho^*$, $\xi_c\simeq D(\rho_0-\rho^*)^{-(n-1)}$. For $\rho_0<\rho^*$ the bulk density is equal to the boundary density at $x=0$. Coming from the boundary at $x=L$, the profile approaches its bulk value exponentially on a length scale $\xi=D/c$, where $c=j'(\rho_0)>0$. It will become clear later that c is a characteristic drift velocity for the density fluctuations. On approaching the transition at $\rho_0=\rho^*$, ξ diverges as $(\rho^*-\rho_0)^{-(n-1)}$. Hence the transition occurs between a phase with a characteristic length scale ξ and a scale-invariant power-law phase. Preliminary investigations of spatial correlations [11] indicate that they behave qualitatively similar to the density profile. We note that ξ and the crossover scale ξ_c diverge with the same exponent as $\rho_0\to\rho^*$.

Up to now we have neglected the effects of fluctuations on the diffusion constant D. This is justified only in dimensions $d\geq 3$. For $d\leq 2$, the leading quadratic nonlinearity in the expansion of $j(\rho)$ around the bulk density is a relevant perturbation which leads to superdiffusive spreading of density fluctuations [7,8], and hence to a scale-dependent diffusion constant. In one dimension the exact scaling form for the fluctuations implies [7,8] that $D\sim(\text{length})^{1/2}$. It is then natural to try to incorporate fluctuations by simply replacing D by the square root of some appropriate length scale in the expressions derived from the "mean-field" equation (2). Specifically, the density profile in the generic case $n=2$ is then predicted to decay as $x^{-1/2}$ and the length scales ξ and ξ_c diverge as $|\rho_0-\rho^*|^{-2}$ on approaching the transition. For $\rho_0>\rho^*$ this implies the scaling form

$$\rho(x)-\rho^*=(\rho_0-\rho^*)F(x(\rho_0-\rho^*)^2)\,, \tag{3}$$

where $F(0)=1$ and $F(x)\sim x^{-1/2}$ for $x\to\infty$. Surprisingly, this simple minded ansatz is well borne out by the simulation results depicted in Fig. 3. In two dimensions the effect of fluctuations is marginal [7,8], and is expected to lead to logarithmic corrections to the mean-field profiles. In that sense $d=2$ is the upper critical dimension of the problem. As a consequence of the fluctuations, the excess current in a finite one-dimensional system is of the order [12] $1/L$ for $\rho_0>\rho^*$ and the bulk density gradient is $O(L^{-3/2})$ rather than $O(1/L^2)$ as predicted by (2). For $\rho_0<\rho^*$ these quantities are exponentially small in L. Numerical results confirming this will be presented elsewhere.

A second type of phase transition is associated with qualitative changes in the current-density relation $j(\rho)$.

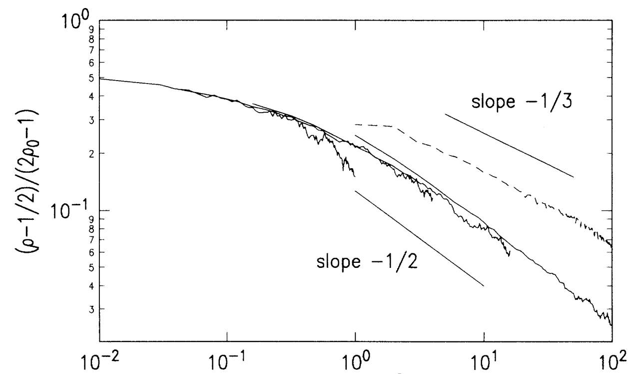

FIG. 3. Density profiles scaled according to (3) with $\rho^*=\frac{1}{2}$. The solid curves correspond to $\beta=0$ and $\rho_0=1$, 0.7, 0.6, and 0.55; the dashed curve corresponds to $\beta=\beta_c$ and $\rho_0=1$. System size and statistics are as in Fig. 1.

Consider a one-dimensional lattice gas with repulsive nearest-neighbor interactions [13]. As before, the motion of particles is restricted to nearest-neighbor hops in the positive x direction, but jumps which increase the number of pairs of occupied nearest-neighbor sites are suppressed by an exponential factor $e^{-\beta}$, where β plays the role of reduced inverse temperature. Hence for large β the current at half filling, $\rho=\frac{1}{2}$, will be strongly suppressed, while away from $\rho=\frac{1}{2}$ a finite current can flow without changing the number of nearest-neighbor pairs. Since obviously $j(0)=j(1)=0$ for all β, this implies that the current develops a double-hump structure [14] when β exceeds some critical value β_c, with two degenerate maxima at densities $\rho_1(\beta)$ and $\rho_2(\beta)$, $\rho_1>\rho_2$. In the limit $\beta\to\infty$ the calculation of the current can be related to the one-dimensional dimer problem [15], which yields the exact result $\lim_{\beta\to\infty}\rho_{1,2}(\beta)=\frac{1}{2}\pm(\sqrt{2}-1)/2$.

Using (1) and (2) it follows that a current-density relation with two degenerate maxima leads to a density profile with two plateaux at densities ρ_1 and ρ_2 separated by an interface, provided that $\rho_0>\rho_1$ (Fig. 1). The position of the interface is determined by the ratio $j''(\rho_1)/j''(\rho_2)$. For symmetric maxima the interface is located at $x=L/2$ on average. Within the mean-field description (2) the interface width is proportional to D; hence it is expected to be roughened by fluctuations in dimensions $d\leq 2$. As ρ_0 is lowered past ρ_1 a transition occurs to a profile with a single plateau at density ρ_2. This transition is of first order in the sense that the spatially averaged density jumps from $\bar{\rho}=\frac{1}{2}$ to $\bar{\rho}=\rho_2$ at $\rho_0=\rho_1$.

The resulting phase diagram in the $(\rho_0,1/\beta)$ plane is summarized in Fig. 4. The diagram was obtained by using a specific choice of jump rates [1] which permits the current-density relation to be computed exactly for all values of β [16]. Increasing β at fixed $\rho_0>\frac{1}{2}$ the phase separation into two plateaux occurs at $\beta_c=2\ln 3$. The transition is continuous and $\rho_1-\rho_2\sim(\beta-\beta_c)^{1/2}$ as in classical Landau theory. At the transition point the current has a maximum of order $n=4$, and (2) predicts a $x^{-1/3}$ decay of the density profile. Since the relevant quadratic nonlinearity [7,8] is absent at $\beta=\beta_c$, the fluctuations are not expected to change this behavior, in agreement with the numerical results depicted in Fig. 3. Close to the transition, $\beta\lesssim\beta_c$, the profile crosses over from $x^{-1/3}$ to $x^{-1/2}$ decay on a length scale $\xi_c\sim\lambda^{-3/2}$, where $\lambda=j''(\frac{1}{2})\sim\beta_c-\beta$.

It is worth pointing out that, in the particular case shown in Fig. 4, the total current J at $\rho_0>\rho_1$ decreases only slightly from $J=\frac{1}{8}$ at $\beta=\beta_c$ to $J=(\sqrt{2}-1)^2/2$ at $\beta=\infty$ (without any discernible feature at β_c) although the current at half filling becomes exponentially small in β. This illustrates rather strikingly how the current maximization principle (1) drives the phase separation: The nonuniform density profile allows the system to maintain a large current despite the presence of interactions which tend to suppress the particle motion. Possibly a similar mechanism could be invoked to explain the patterns observed recently in simulations of a two-dimensional lattice gas with attractive interactions and open boundaries [5]. Indeed a significant increase in the current, as compared to the system with periodic boundary conditions, was observed in these simulations.

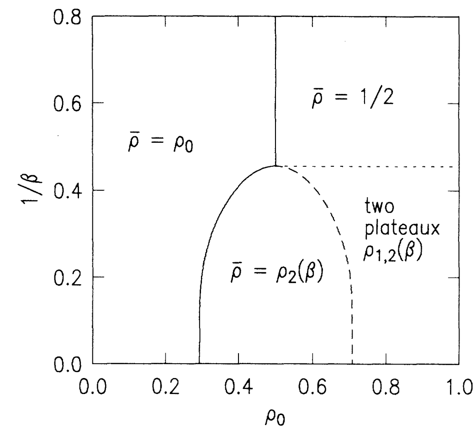

FIG. 4. Phase diagram for the one-dimensional lattice gas with repulsive interactions. The solid and dotted lines denote the two types of continuous transitions and the dashed line denotes a discontinuous transition.

Having elucidated the behavior of the average density profile in various regimes, the natural next step is to consider spatiotemporal correlations. In general, this is a difficult task, since it involves expanding around a nonuniform profile which itself is not explicitly known [11]. Here I concentrate on the most easily accessible quantity, the frequency spectrum of the particle number fluctuations [17], and I assume a single-humped current-density relation. Separating the fluctuations from the average density profile through $\rho=\langle\rho\rangle+\phi$, $\langle\phi\rangle=0$, and approximating the average profile by a constant, $\langle\rho\rangle=\bar{\rho}$, we obtain a fluctuating Burgers equation [7,8] for ϕ with a drift term $c\,\partial\phi/\partial x$, $c=j'(\bar{\rho})$, and a nonlinearity $\lambda\phi\,\partial\phi/\partial x$, $\lambda=j''(\bar{\rho})$. We ignore the boundary conditions for the fluctuations and treat the finite system as a slab of an infinitely extended system [18]. The particle number fluctuations are then readily calculated and we find a spectrum $\langle|N(\omega)|^2\rangle\sim\omega^{-\alpha}$ for $L\to\infty$. For $c\neq 0$ the exponent $\alpha=2$, while for $c=0$ the value depends on dimension and the presence of the nonlinearity. For $\lambda\neq 0$, $\alpha=\frac{3}{2}$ in $d\geq 2$ with logarithmic corrections in $d=2$, and [7] $\alpha=\frac{5}{3}$ in $d=1$; for $\lambda=0$, $\alpha=\frac{3}{2}$ in all dimensions. This result once more illustrates the different nature of the phases $\rho_0>\rho^*$ and $\rho_0<\rho^*$. In the latter case $c\neq 0$, which not only provides a length scale $\xi=D/c$ for the decay of correlations, but also leads to a linear drift of density fluctuations through the system which generates trivial $1/\omega^2$ number fluctuations. In the power-law phase, $c=0$ and the number fluctuation spectrum reflects the internal (diffusive or superdiffusive) dynamics of the system. The predictions for α have been verified by simulations in one dimension for $\beta=0$ and $\beta=\beta_c$ (where $\lambda=0$). Note that generically the condition $c=0$ would have to be achieved by fine tuning of parameters. The fact that it is maintained by the boundary conditions over a finite range of boundary densities ρ_0 may thus be regarded [19] as an example of self-organized criticality [20].

In conclusion, I have presented a detailed study of driven diffusive systems with open boundaries, and demonstrated dramatic boundary effects which are quite unexpected from the point of view of equilibrium statistical mechanics. It should be noted that the boundary conditions employed in this work are rather more realistic physically than the ring geometry used in most previous studies [1-4], thus the effects described here should be accessible to experiments. Theoretically, it would be of interest to explore how the boundary-induced phase transitions can be embedded into an equilibrium context using the mapping [21] of one-dimensional diffusive particle systems onto two-dimensional vertex models. Finally, I hope that my results will prove to be useful in future investigations of other nonequilibrium stationary states in which boundary conditions play a prominent role [5,10,17,20].

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