Extremal principle for the steady-state selection in driven lattice gases with open boundaries

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(Received 5 September 2000; published 23 May 2001)

This paper investigates the steady states of one-dimensional driven lattice gases with open boundary conditions. It shows how the extremal principle proposed recently by Popkov and Schütz can be modified to apply to more general cases. Monte Carlo simulations are presented for a one-dimensional totally asymmetric simple exclusion process with nearest neighbor repulsion under parallel update as an example. The simulations enable one to guess the exact phase diagram for this particular lattice gas with deterministic bulk dynamics, by fitting the data to analytic formulas, which appear to be exact in the thermodynamic limit.

DOI: 10.1103/PhysRevE.63.067103 PACS number(s): 05.70.Fh, 05.70.Ln, 02.50.Ga

Driven diffusive lattice gases serve as simplified models for a wide variety of problems, just to mention traffic flow [1], kinetics of protein synthesis [2], and fast superionic conductors [3]. One-dimensional driven lattice gases like the asymmetric simple exclusion process (ASEP) provide more convienient prototypes to study genuine nonequilibrium behavior, since they are easy to simulate and there is considerable recent progress in analytic solutions of specific models [4]. Ion diffusion in zeolites [5] and single file diffusion of colloid particles in narrow channels [6] are interesting experimental realizations of one-dimensional diffusive systems. In the sequel I consider a gas of identical particles with hardcore repulsion on a one-dimensional lattice, subject to short range interactions and to a local conservation law, driven to the right by some kind of external field. The specific example, I am dealing with in the Monte Carlo (MC) simulations, is defined by the transition rules (4) [7].

For periodic boundary conditions a genuine driven one-dimensional lattice gas approaches a steady state of constant density ρ with some constant nonequilibrium current $j(\rho)$. In the limit of large system size the current density (CD) relation $j(\rho)$, measured in systems with fixed density and periodic boundary conditions, characterizes the bulk behavior of the model under consideration and shows up, e.g., as fundamental diagram in traffic flow. Clearly $j(0)=j(1)=0$ due to a total lack of particles resp. holes and for the most simple models, like the ASEP $j(\rho)$ has a single maximum in between. In general the CD relation may have several maxima with additional minima in between (see Fig. 1 for a example). Krug [8] asked for the emerging steady state for gas with given CD relation $j(\rho)$ and given injection rates $\{\alpha\}$ and drainage rates $\{\beta\}$. He partially answered the question by proposing a maximum principle for the nonequilibrium current: $j=\max_{\rho\in[0,\rho_0]}j(\rho)$. The steady state is the maximum of the CD relation $j(\rho)$ over the interval $[0,\rho_0]$, where the boundary density is ρ_0 at the left side and zero at the right side. Here the boundary densities were the mean densities at the leftmost and rightmost lattice site. For simple examples with an injection rate α and a drainage rate β there exist monotonous relations between these boundary densities and the rates, e.g., $\rho_-=\alpha$ and $\rho_+=1-\beta$ for the ASEP. So one can plot the phase diagram equally well in terms of the rates α and β or in terms of the boundary densities. For more complicated models we may have a whole set of microscopic injection and drainage rates $\{\alpha\}=\{\alpha_1,\alpha_2,\dots\}$ and $\{\beta\}=\{\beta_1,\beta_2,\dots\}$, which may vary independently, so that it is unfeasible to plot the high dimensional phase diagram in terms of only two boundary densities. Due to this fact I use the microscopic rates as variables in plots of phase diagrams.

Based on work [9], that explains the phase diagram of the ASEP in terms of the collective velocity

$$v_c=\frac{\partial j(\rho)}{\partial\rho}, \tag{1}$$

describing the propagation of a local perturbation in a system with constant density ρ, and the shock velocity

$$v_s=\frac{j_+-j_-}{\rho_+-\rho_-}, \tag{2}$$

of a shock with limiting densities ρ_+ and ρ_-, Popkov and Schütz [10] proposed the extremal principle

$$\begin{aligned} j&=\max_{\rho\in[\rho_+,\rho_-]} j(\rho) \quad \text{for} \quad \rho_->\rho_+ \\ j&=\min_{\rho\in[\rho_-,\rho_+]} j(\rho) \quad \text{for} \quad \rho_-<\rho_+, \end{aligned} \tag{3}$$

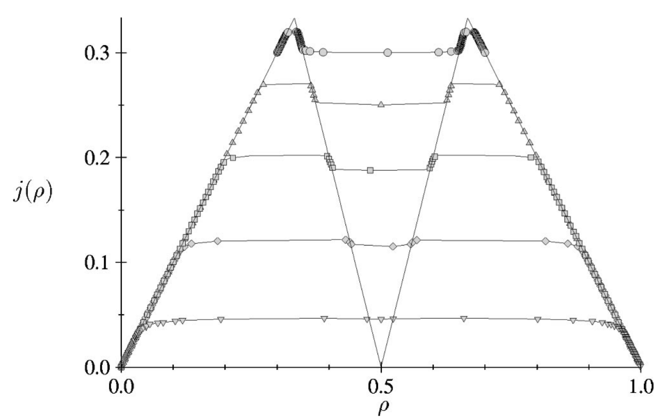

FIG. 1. Bulk CD relation $j(\rho)$ for deterministic bulk dynamics $(p=0)$ together with MC data for open boundary conditions taken along lines with boundary rates $\alpha=c-\beta$ for $c=1.5,1.0,0.6,0.3,0.1$ from top to bottom.

with left boundary density ρ_- and right boundary density ρ_+. For CD relations with two maxima this principle predicts a new minimal current phase that was confirmed by MC simulations [10]. Recently, Antal and Schütz [11] presented data for a lattice gas with attractive interactions that contained an additional phase not predicted by the extremal principle (3), when using boundary densities $\rho_-=\alpha$ and $\rho_+=1-\beta$, while the rest of the phase diagram was predicted faithfully. This casts some doubt on the general validity of Eq. (3). In the sequel I discuss MC data for another one-dimensional lattice gas, where the minimal current phase is absent. The goal of this paper is then to interpret Eq. (3) in a way that the aforementioned cases can be included.

Let us consider a lattice gas of particles driven to the right according to the rules

$$\begin{aligned}
&1100\rightarrow 1010 \quad \text{with probability } 1-p,\\
&1101\rightarrow 1011 \quad \text{with probability } 1-p,\\
&0100\rightarrow 0010 \quad \text{with probability } 1-p,\\
&0101\rightarrow 0011 \quad \text{with probability } p,
\end{aligned} \tag{4}$$

where $p\in[0,1]$. The CD relation for deterministic bulk dynamics at $p=0$ is plotted in Fig. 1. Recently a rigorous derivation of its shape was given [12]. A small but finite $p>0$ leads to a current density relation with differentiable extrema and decreased currents for the maxima but a increased current $j_{min}>0$ for the minimum. Note that for $p=1/2$ the model is just the totally asymmetric simple exclusion process under a parallel stochastic update with a single humped parabolic CD relation. For some value of p in between the minimum in the CD relation vanishes. We first discuss the deterministic case $p=0$ and afterwards check the influence of stochastic parallel dynamics for a value of $p=0.0625$. The nearest neighbor repulsion leads to a zero current state (. . . 010101 . . .) at density $\rho=1/2$. Using a deterministic parallel update leads to a piecewise linear CD relation with maximal current $j=1/3$ for the densities $\rho=1/3$ and $\rho=2/3$ and zero current for $\rho=0,1/2,1$ (see Fig. 1). The creation rates $\{\alpha\}$ at the left boundary and the annihilation rates $\{\beta\}$ at the right boundary are chosen as

$$\begin{aligned}
&1|00\rightarrow 1|10 \quad \text{with probability } \alpha,\\
&1|01\rightarrow 1|11 \quad \text{with probability } \alpha,\\
&11|0\rightarrow 10|0 \quad \text{with probability } \beta,\\
&01|0\rightarrow 00|0 \quad \text{with probability } \beta.
\end{aligned} \tag{5}$$

The hopping rates of the leftmost and the next to rightmost site are governed by the bulk rules in conjunction with the constant dummie boundary sites added in Eq. (5). Note that the automaton is symmetric under interchange of A and 0, combined with a reversion of the driving direction. Our choice of boundary conditions renders the minimal current state $j(1/2)=0$ at density $\rho=1/2$ unstable and thereby destroys the minimal current phase.

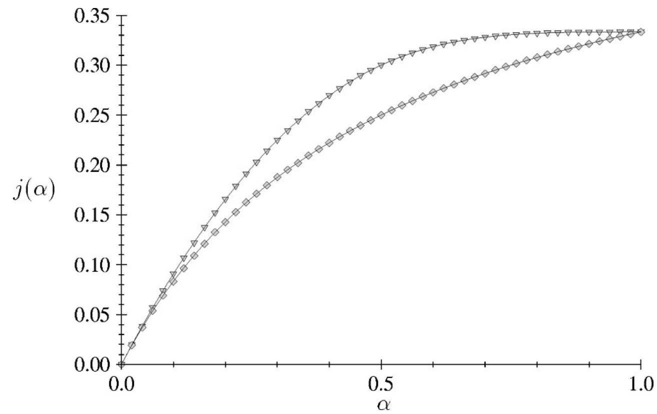

FIG. 2. Steady-state currents in a ''semi-infinite'' system for deterministic bulk dynamics as functions of the injection rate α. The upper curve (triangles) is $j_{(0)}(\alpha)$ for an initially empty system and the lower curve (diamonds) is $j_{(1/2)}(\alpha)$ for a system prepared initially in the current zero state with density 1/2. Symbols denote MC data and full lines analytical fits as given in the text.

I simulated a system of size $L=5600$ upto 10^6 time steps to obtain averages for current and density after an initial 10^5 time steps necessary to reach the steady state. The results of the simulations are displayed in Figs. 1–3. Figure 2 shows the steady-state currents for a system loaded with rate α, when the left boundary determines the steady state. The upper curve (triangles) is the resulting current $j_{(0)}(\alpha)$ when one fills an initially empty system, setting $\beta=1$ at the right boundary. The lower curve (diamonds) is the resulting current $j_{(1/2)}(\alpha)$, where initially the zero current state (. . . 010101 . . .) was prepared and stabilized by forbidding

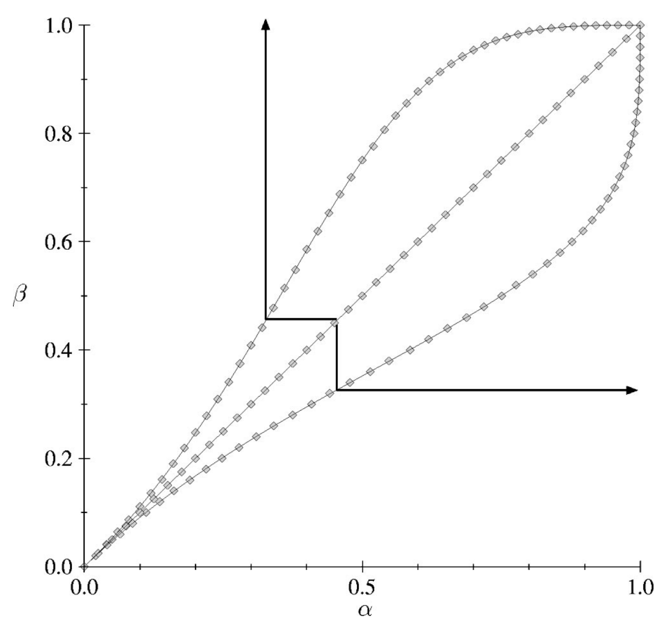

FIG. 3. Phase diagram for deterministic bulk dynamics as a function of the injection rate α and the drainage rate β. Diamonds denote the MC data for the first order transitions and the connecting lines denote the analytical fits. The full line with two arrows follows a typical path of constant current and density, but with density jumps at the phase transitions.

the process $01|0 \rightarrow 00|0$, while allowing the $11|0 \rightarrow 00|0$ with probability 1 at the right boundary. The boundary conditions of the right side were choosen in a way that no shock traveled from the right to the left boundary for any value of α, to mimic the behavior of a semi-infinite system. Inspired by the result of the analytical solution for an ASEP with fully parallel update [13] I conjectured the following analytical forms for the currents:

$$j_{(1/2)}(\alpha) = \frac{\alpha}{1+2\alpha}, \quad j_{(0)}(\alpha) = \frac{\alpha - \alpha^2 + \alpha^3}{1+2\alpha^3}. \tag{6}$$

In Fig. 2 these formulas are plotted as full lines, which perfectly fit the MC data denoted by symbols. It turns out that these two currents are enough to construct the phase diagram displayed in Fig. 3. I find three lines of first order transitions between low density phases where α determines the bulk density $\rho = \rho_-(\alpha)$ and the steady-state current $j(\alpha)$, and high density phases, where β determines these values. Along the line $\alpha = \beta$, the current is equal to $j_{(1/2)}(\alpha)$, while it is equal to $j_{(0)}(\alpha)$ along the line $\beta = 1$. Together with the condition that the current is continous at the transition this enables us to derive the analytical expression

$$\beta = \frac{\alpha - \alpha^2 + \alpha^3}{1 - 2\alpha + 2\alpha^2}, \tag{7}$$

for the upper curved transition line in Fig. 2, simply by equating the two currents of Eq. (6) with $\alpha = \beta$ in $j_{(1/2)}(\alpha)$. The lower line then follows by symmetry. I expect Eqs. (6) and (7) and corresponding formulas for the density ρ, which follow via the CD relation, to be exact analytical results in the thermodynamic limit. Figure 1 displays, besides the bulk CD relation measured in systems with periodic boundary conditions, MC data for $j(\rho)$ taken along lines $\alpha = c - \beta$ for $c = 1.5, 1.0, 0.6, 0.3, 0.1$ from top to bottom. The data lie, modulo finite size effects, on the bulk CD relation but exhibit density jumps at the transition lines, while the current is continous.

How can we explain these findings in accordance with the extremal principle (3)? The crucial question is how the ''boundary'' densities ρ_- and ρ_+ are defined. For the ASEP it is possible to take the reservoir densities α and $1-\beta$, but this turns out to be inadequate for more complicated systems. As it stands Eq. (3) tells us about the evolution of a shock with limiting densities ρ_- and ρ_+ [10]. In the case $\rho_- < \rho_+$ we have $v_s > 0$ for $j_+ > j_-$ and $v_s < 0$ for $j_+ < j_-$, i.e., the region of smaller current grows and vice versa for $\rho_- > \rho_+$. In addition if there is a minimum of $j(\rho)$ in the interval $[\rho_-, \rho_+]$ the shock will be unstable and split into two shocks with limiting densities ρ_-, ρ_{min} and ρ_{min}, ρ_+, evolving to the left resp. right, thereby creating the minimal current phase. Such a steady state we may call bulk dominated. Similar considerations apply for the case $\rho_- > \rho_+$, where a maximal current phase can occur. But how are ρ_- and ρ_+ connected to the microscopic boundary conditions $\{\alpha\}$ and $\{\beta\}$? Due to the short range nature of the interactions one expects $\rho_-(\{\alpha\})$ to be a function only of the $\{\alpha\}$ and of bulk properties. Any influence of the $\{\beta\}$ must be mediated by the bulk state $[\rho, j(\rho)]$ via a shock as explained above. Thus $\rho_-(\{\alpha\})$ contains all the bulk densities of a semi-infinite system that are supported (or controlled) by some value of the rates $\{\alpha\}$. This can be only bulk densities where $v_c > 0$ so that a perturbation caused by a small change of the $\{\alpha\}$ can spread into the bulk. In addition I include bulk dominated regions where ρ and j are constant under variation of α into $\rho_-(\{\alpha\})$ and $j_-(\{\alpha\})$ if they can be reached by tuning the rates $\{\alpha\}$.

For every lattice gas with a single hump in the CD relation this choice implies that one has always $\rho_- < \rho_+$ and therefore only the minimization part of Eq. (3) is needed. If the maximum current phase occurs it is already contained in the relations $\rho_-(\{\alpha\})$ and $\rho_+(\{\beta\})$. The advantage of this choice of ρ_- and ρ_+ is, that the reentrance transition observed in [11] is now predicted by Eq. (3) since ρ_+ in our definition, after reaching the maximal current phase from above with further increase of the drainage rate β increases again. The minimization part of Eq. (3) then prefers ρ_+ instead of the maximal current phase offered by the injection side.

Generally the relations $\rho_-(\{\alpha\})$ and $\rho_+(\{\beta\})$ have some nonuniversal dependence of the microscopic transition rates, as the CD relation itself depends on the bulk transition probabilities, and they are needed as input to determine the phase diagram via Eq. (3). In our example the bulk CD relation has two branches with $v_c > 0$ so $\rho_-(\{\alpha\})$ and $j_-(\{\alpha\})$ can be double valued relations that is indeed the case for our choice of boundary conditions, as can be seen in Fig. 2. For a given set of $\{\alpha\}$ and $\{\beta\}$ we have to put all four combinations of $\rho_{-(0)}(\{\alpha\})$, $\rho_{-(1/2)}(\{\alpha\})$, $\rho_{+(0)}(\{\beta\})$, and $\rho_{+(1/2)}(\{\beta\})$ in Eq. (3). This leads to

$$\min\{j(\rho_{-(0)}(\alpha)), j(\rho_{+(0)}(\beta))\}, \tag{8}$$

$$\min\{j(\rho_{-(0)}(\alpha)), j(\rho_{+(1/2)}(\beta))\}, \tag{9}$$

$$\max\{j(\rho_{+(1/2)}(\beta)), j(\rho_{-(1/2)}(\alpha))\}, \tag{10}$$

$$\min\{j(\rho_{-(1/2)}(\alpha)), j(\rho_{+(0)}(\beta))\}, \tag{11}$$

where just the smaller or larger of both currents is chosen. Extremalization on the whole interval $[\rho_-, \rho_+]$ as in Eq. (3) is not necessary since the extremal current phases selected thereby are already contained in our definition of the densities. The conditions (8)–(11) determine unambigously the phase diagram of Fig. 3. Presumably, Eqs. (8)–(11) are sufficient to determine the phase diagram for all double humped CD relations. Note that in our model there is $j(\rho_{-(0)}(\alpha)) > j(\rho_{-(1/2)}(\alpha))$ for all α and $j(\rho_{+(0)}(\alpha)) > j(\rho_{+(1/2)}(\alpha))$ for all β. Thus Eqs. (9)–(11) imply (8). Figure 3 lacks any kind of extended bulk dominated extremal current phases. This has slightly different reasons for the maximal current phases and the minimal current phase. The lack of maximal current phases clearly is due to the deterministic bulk dynamics, which prevents the necessary overfeeding effect [7,14]. Such phases immediately appear if one allows for probabilities $p < 1$ in Eq. (4). The absence of the minimal current phase is,

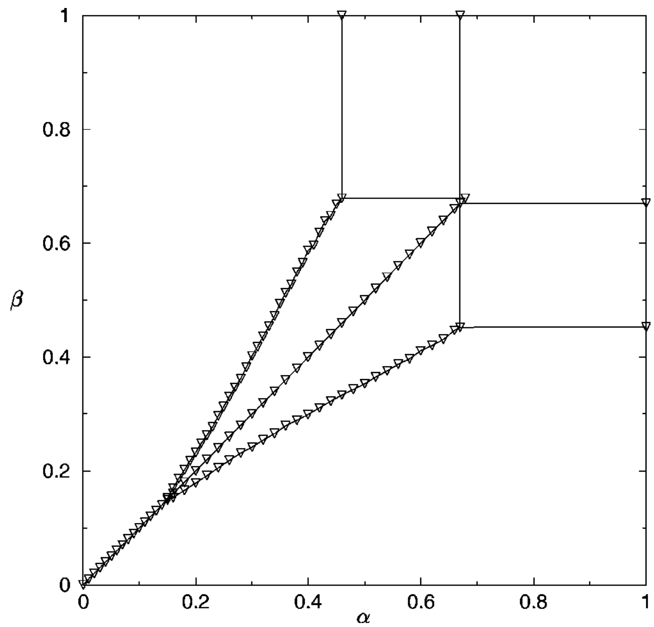

FIG. 4. Phase diagram for stochastic bulk dynamics ($p = 0.0625$) as a function of the injection rate α and the drainage rate β. Diamonds denote the MC data for the phase transitions.

as we have seen, due to the fact, that it is instable for our choice of boundary conditions. To check these claims I performed simulations with a stochastic parallel update setting $p = 0.0625$. Figure 4 displays the phase diagram, again measured for $L = 5600$. Three different maximal current phases appear in the rectangles visible in the upper right corner. The off diagonal ones contain the two pure maximal current phases of high and low density. The diagonal one contains both maximal current phases separated by a diffusing shock and thereby marks the area (instead of a line), where the first order transition between the pure maximal current phases occur (see remark [16] of [10]). In contrast the minimal current phase is still restricted to the single point in the lower left corner of Fig. 4, where four lines of first order transitions meet. To stabilize it in a finite range one has to supress the processes $1|01 \rightarrow 1|11$ and $01|0 \rightarrow 00|0$ at the boundaries. The phase diagram of Fig. 4 can be obtained by applying Eqs. (8)–(11) to the apropriate currents measured in ''semi-infinite'' systems. In conclusion I showed how the phase diagram of some one-dimensional lattice gases with open boundaries can be obtained by the extremal principle (3). We argued that the boundary densities used in Eq. (3) are the bulk densities of a semi-infinite system and that they are restricted to densities, where the collective velocity v_c allows a perturbation by the boundary to move into the bulk. The continous transitions to a extremal current phase are already present in these boundary densities, while the first order transition mediated by a shock of finite height are determined by Eqs. (8)–(11). More complicated systems are likely to lead to new surprises, just to mention systems with inhomogenious steady states, which occur frequently in higher dimensions [15] but also in one-dimensional two species systems with spontaneously broken symmetry [16].

I am grateful to Gunter Schütz for suggesting the problem, numerous useful discussions and for a lot of comments on the manuscript and to Joachim Krug for a critical reading of the manuscript. This work was partially supported by SFB 237 Unordnung und grosse Fluktuationen.

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