Localization of shocks in driven diffusive systems without particle number conservation

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We study the formation of localized shocks in one-dimensional driven diffusive systems with spatially homogeneous creation and annihilation of particles (Langmuir kinetics). We show how to obtain hydrodynamic equations that describe the density profile in systems with uncorrelated steady state as well as in those exhibiting correlations. As a special example of the latter case, the Katz-Lebowitz-Spohn model is considered. The existence of a localized double density shock is demonstrated in one-dimensional driven diffusive systems. This corresponds to phase separation into regimes of three distinct densities, separated by localized domain walls. Our analytical approach is supported by Monte Carlo simulations.

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I. INTRODUCTION

One-dimensional driven diffusive systems proved to be a rewarding research topic in the past years [1]. They were shown to exhibit boundary induced phase transitions [2], spontaneous symmetry breaking [3,4] and phase separation [5,6]. Recently, the case of systems without particle conservation in the bulk attracted attention. In Ref. [7], the effect of a single detachment site in the bulk of an asymmetric simple exclusion process (ASEP) was studied. In Refs. [8,13], the interplay of the simplest one-dimensional driven model, the totally asymmetric exclusion process (TASEP) with local absorption/desorption kinetics of single particles acting at all sites, termed "Langmuir kinetics" (LK) was considered. These models were inspired by the dynamics of motor proteins [22], which move along cytoskeletal filaments in a certain preferred direction while detachment and attachment can also occur between the cytoplasm and the filament, and, in a very different setting, by dynamics of limit orders in a stock exchange market. Being an equilibrium process, LK is well understood, while the combined process of TASEP and LK showed the new feature of a localized shock in the density profile of the stationary state [8].

The TASEP is defined on a one-dimensional lattice of size L. Each site can either be empty or occupied by one particle. In the bulk, particles can hop from site i to site $i+1$ with unit rate, provided the target site is empty. At site 1, particles can enter the lattice from a reservoir with density ρ_-, provided the site is empty. They can leave the system from site L into a reservoir of density ρ_+ with rate $1-\rho_+$. Thus in the interior of the lattice, the particle number is a conserved quantity. The phase diagram and steady states of the TASEP as a function of the boundary rates are known exactly [9–11]. Furthermore, a theory of boundary induced phase transitions exists, which explains the phase diagram quantitatively in terms of the dynamics of shocks [12]. In the stationary state, these shocks exist as an upward density shock along the coexistence line between the high- and the low-density phases, i.e., they connect a region with low density to the left of the shock position with a high-density region to its right. The shock performs a symmetric random walk between the boundaries of the system.

One may equip the system with the additional feature of local particle creation at empty sites with rate ω_a and annihilation with rate ω_d (see Fig. 1) [8,13]. In the thermodynamic limit $L\rightarrow\infty$, there are three regimes to be distinguished. If ω_a and ω_d are of an order larger than $1/L$, the steady state of the system will be that of Langmuir kinetics, i.e., there will be a uniform density of $K=\omega_a/(\omega_a+\omega_d)$ in the system. In case of ω_a and ω_d being of smaller order than $1/L$, the local kinetics is negligible and the system will behave as the TASEP. The case of the local rates being of the order of $1/L$ is the most interesting one, and will be investigated further on. Writing

$$\omega_a=\Omega_a/L, \quad \omega_d=\Omega_d/L, \tag{1}$$

the phase diagram can be formulated in terms of Ω_a, Ω_d, ρ_-, and ρ_+. In Ref. [8], it was shown that for Ω_a and Ω_d fixed, the phase diagram as a function of ρ_- and ρ_+ does not only exhibit the low-density and high-density phases known from the TASEP, but also a high-low coexistence phase. In this phase, the shock does not move in the system but its position is a function of the rates ρ_- and ρ_+ (see Fig. 2).

Parmeggiani *et al.* presented not only Monte Carlo simulations, but derived also a mean field equation for the density profile which was shown to coincide with the simulation profiles. We argue here that the mean field approximation cannot be used in general. The coincidence with the Monte Carlo (MC) simulations in Ref. [8] is due to lack of correlations in true steady state of the TASEP. We claim that the stationary density profile can be derived, in general, using a hydrodynamic equation and taking correlations into account (in case of the TASEP, this equation is equal to that obtained with a mean field approach). For the Katz-Lebowitz-Spohn (KLS) model, which is a generic model of interacting driven diffusive systems [14,15], we show that this hydrodynamic equation correctly describes the density profiles on a quantitative level, while a mean field approach would fail to repro-

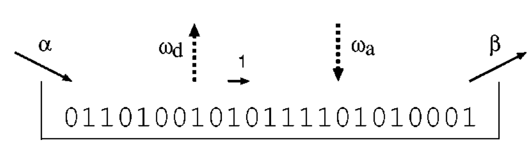

FIG. 1. Possible processes and their rates in the model of the ASEP with Langmuir kinetics.

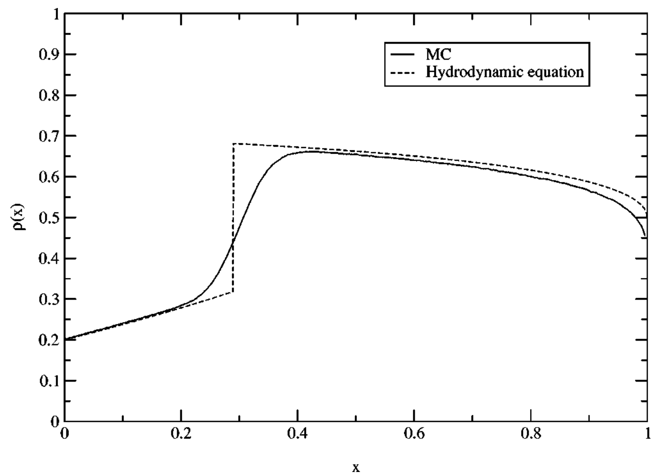

FIG. 2. Plot of an average density of particles ρ versus rescaled coordinate x (*site number/L*) of a localized density shock in the ASEP with Langmuir kinetics. Parameters are $\rho_-=0.2$, $\rho_+=0.6$, $\Omega_a=0.3$, and $\Omega_d=0.1$. We show the results of both Monte Carlo simulations for $L=1000$ and the mean field approach.

duce even the basic qualitative features of the system, e.g., phase separation into three distinct density regimes.

II. HYDRODYNAMIC EQUATION

In the following, we are interested in the $L\to\infty$ limit in which we rescale lattice spacing $a=1/L\to 0$ and time $t=t_{\mathrm{lattice}}/L$ (Eulerian scaling) to get the continuous (hydrodynamic) limit of the model. In this framework, $\Omega_{a,d}$ are the attachment/detachment rates per unit length. We claim that the hydrodynamic equation describing the time dependence of the local density $\rho(x)$ for a general driven diffusive system with Langmuir kinetics takes the form

$$\frac{\partial}{\partial t}\rho+\frac{\partial}{\partial x}j(\rho)=\mathcal{L}(\rho), \tag{2}$$

where $j(\rho)$ is the *exact* current in a driven diffusive system with homogeneous density ρ without LK and $\mathcal{L}(\rho)$ is the source term describing the Langmuir kinetics. Here, we consider only that choice of $\mathcal{L}(\rho)$ which corresponds to the process depicted in Fig. 1:

$$\mathcal{L}(\rho)=\Omega_a(1-\rho(x,t))-\Omega_d\rho(x,t). \tag{3}$$

Other choices of $\mathcal{L}(\rho)$, which might, e.g., describe the local annihilation of particle pairs, are to be discussed in a forthcoming publication [16].

As is usually done in the rigorous derivation of the hydrodynamic limit of conservative systems [17], our nonconservative Eq. (2) implicitly assumes that the system is locally stationary because the exact form of the stationary flux is used. We argue that this assumption is justified since the nonconservative part of the dynamics of the system at macroscopic scale is so slow that locally the system reaches stationarity with respect to the conservative part of the dynamics. Any finite perturbation caused by the nonconservative dynamics would travel a macroscopic distance and hence dissipate before interacting with another perturbation. Hence the hydrodynamic description (after time rescaling $t\to\epsilon t$) is adequate for describing the full dynamics. For physical insight in the formation of shocks, one needs other tools which are discussed below.

Rewriting Eq. (2) by using $\partial_t\rho(x,t)=0$ in the stationary state, and $\partial_x j=\partial j/\partial\rho\cdot\partial\rho/\partial x$ yields for the stationary density profile $\rho(x)$:

$$v_c(\rho)\frac{\partial\rho(x)}{\partial x}=\mathcal{L}(\rho). \tag{4}$$

Here, $v_c=\partial j/\partial\rho$ is the collective velocity, i.e., the drift velocity of the center of mass of a local density perturbation on a homogeneous stationary background with density ρ (for system with the Langmuir kinetics switched off) [1,12]. The stationary density profile has to satisfy Eq. (4) as well as the boundary conditions $\rho(0)=\rho_-$ and $\rho(1)=\rho_+$. As Eq. (4) is of first order there will be, in general, no smooth solution fitting both boundary conditions. In the original lattice model, this discrepancy is resolved by the appearance of shocks and/or boundary layers. To regularize the problem, one can add to Eq. (2) and correspondingly to Eq. (4) a vanishing viscosity term

$$v_c(\rho)\frac{\partial\rho(x)}{\partial x}=\mathcal{L}(\rho)+\nu\frac{\partial^2\rho(x)}{\partial x^2}, \tag{5}$$

where $\nu>0$ is of the order of $1/L$. This term makes the hydrodynamic equation of second order, and ensures a smooth solution fitting both boundary conditions. The shock has then a width of the order of $1/L$ (see Ref. [8]), i.e., in the thermodynamic limit the rescaled solution becomes discontinuous. We claim that Eq. (5) gives the same result in the $L\to\infty$ limit as the Monte Carlo simulations, therefore it can be used as a tool to compute the stationary density profile. The main difference between Eq. (5) and the MC simulations is that the former does not take fluctuations into account, which leads to a shock width of the order of $1/L$, while in a MC simulations after averaging it is of the order of $1/\sqrt{L}$ due to the fluctuation of the shock position.

The stationary density profile for a given $j(\rho)$ and parameters Ω_a, Ω_d, ρ_-, and ρ_+ can be derived from the flow field of the differential equation (4) by using the rules formulated and explained below.

(a) In the interior of the lattice, the stationary density profile either follows a line of the flow field of the differential equation (4) or makes a jump. Jumps can only occur between densities yielding the same current, i.e., *the current is continuous in the interior of the lattice*.

(b) Let $\rho'_\pm$ be defined as limiting left and right densities with the boundary layers cut away:

$$\rho'_-=\lim_{x\to+0}\rho(x),\quad \rho'_+=\lim_{x\to 1-0}\rho(x),$$

where $\rho(x)$ is the stationary profile in the hydrodynamic limit. The boundary layer at $x=0$ (i.e., if $\rho_-\neq\rho'_-$) has to satisfy the following condition:

$$\text{if} \quad \rho_- < \rho'_- \quad \text{then} \quad j(\rho) > j(\rho'_-) \quad \text{for any} \quad \rho \in (\rho_-, \rho'_-), \tag{6}$$

$$\text{if} \quad \rho_- > \rho'_- \quad \text{then} \quad j(\rho) < j(\rho'_-) \quad \text{for any} \quad \rho \in (\rho'_-, \rho_-). \tag{7}$$

The condition for the stability of the boundary layer at $x = 1$ (if there is) is similar:

$$\text{if} \quad \rho'_+ < \rho_+ \quad \text{then} \quad j(\rho'_+) < j(\rho) \quad \text{for any} \quad \rho \in (\rho'_+, \rho_+), \tag{8}$$

$$\text{if} \quad \rho'_+ > \rho_+ \quad \text{then} \quad j(\rho'_+) > j(\rho) \quad \text{for any} \quad \rho \in (\rho_+, \rho'_+). \tag{9}$$

(c) Shocks between a density ρ_l to the left of the shock and ρ_r to the right of the shock are stable only if they are stable in the absence of Langmuir kinetics [1,18].

Following are a few remarks pertaining to the rules presented above.

(i) Although LK does not conserve locally the number of particles, Eq. (2) with the vanishing viscosity added (5) can be rewritten formally in the form

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\tilde{j}(x,t) = 0,$$

$$\tilde{j}(x,t) = j(\rho) - \int_A^x \mathcal{L}(\rho)dx - \nu\frac{\partial \rho}{\partial x} - \mathcal{F}(t), \tag{10}$$

where $\mathcal{F}(t)$ is some time-dependent function. Let us suppose that there is a shock at the position X_0 connecting the densities ρ_l and ρ_r. The mass transfer across the shock is

$$\frac{\partial}{\partial t}\int_{X_0-0}^{X_0+0} \rho(x,t)dx = \tilde{j}(X_0+0,t) - \tilde{j}(X_0-0,t) = j(\rho_r) - j(\rho_l), \tag{11}$$

since the Langmuir term and the viscosity term change only infinitesimally across the shock. In the stationary state, the right hand side of Eq. (11) vanishes which explains rule (a).

(ii) Rule (b) is due to the fact that in the boundary layer of vanishing length $\delta l \to 0$, the LK term in Eq. (10) can be neglected. Consequently, for the stationary current at the boundaries, we have $\tilde{j}(x) = j(\rho(x)) - \nu(\partial\rho/\partial x) = J$, which yields the known maximization/minimization principle [1,21] and is equivalent to rule (b). Indeed at the left boundary, $J = j(\rho'_-)$ [see Eq. (6) for notations], and if, e.g., $\rho_- < \rho'_-$, then $(\partial\rho/\partial x) > 0$. Consequently, we obtain $j(\rho_-) = J + \nu(\partial\rho/\partial x) > J$, which is exactly Eq. (6). Analogously one obtains Eqs. (7)–(9).

(iii) Rule (c) is explained by the marginal role the Langmuir kinetics plays locally in both space and time. The first, LK is very slow locally for large L [see Eq. (1)], and the second, it acts ‘‘orthogonally’’ on the particle distribution, not affecting directly the particle motion. Hence, the local perturbations will still spread with the velocity corresponding to the local density level ρ, thus rendering the same stability conditions for a shock as for the diffusive system without LK.

Condition (c) is easy to check geometrically through the current-density relation. An upward (downward) shock is stable if the straight line connecting the points $(\rho_l, j(\rho_l))$ and $(\rho_r, j(\rho_r))$ stays below (above) the $j(\rho)$ curve [18,21]. Because of criterion (a) these lines are always horizontal in this case, which gives zero mean velocity (but not localization) for the shock in absence of Langmuir kinetics.

(iv) In the cases we have considered (ASEP, KLS model), rules (a)–(c) define a unique stable solution (see the Appendix), and we believe that this is true also in general case, i.e., for arbitrary $j(\rho)$ dependence and for the given choice (3) of Langmuir kinetics.

In the following, we apply the general theory to specific models.

III. REVISITING THE ASEP WITH LANGMUIR KINETICS

Using the differential equation (4) and the rules given above, we reconsider the ASEP with Langmuir kinetics [8,13]. Here, the current-density relation is given by $j(\rho) = \rho(1-\rho)$, which yields $v_c(\rho) = 1 - 2\rho$. Thus Eq. (4) becomes

$$(1-2\rho(x))\partial_x\rho(x) = \Omega_a - (\Omega_a + \Omega_d)\rho(x), \tag{12}$$

which is identical with the mean field equation in Ref. [8] in the thermodynamic limit. We would like to stress that this coincidence is caused by the fact that the mean field current-density relation for the TASEP is exact. As is demonstrated below, Eq. (4) also holds when this is not the case, i.e., for the one-dimensional KLS model.

Due to rule (a) as stated above (continuity of the current in the interior of the lattice), shocks in the interior can only occur in the case where $\rho_l = 1 - \rho_r$, as $j(\rho)$ is symmetric to $\rho = 1/2$. Rule (c) (stability of the shock) furthermore requires that $\rho_r > \rho_l$. These observations coincide with the findings of Ref. [8].

We also applied our rules to k-hop exclusion models [19] (with LK added), which are a generalization of the TASEP with stationary product measures and asymmetric current-density relations. Due to this fact shocks appear, which are nonsymmetric with respect to $\rho = 1/2$. MC simulations are in full accord with our predictions [20].

IV. KLS MODEL WITH LANGMUIR KINETICS

A much studied one-dimensional driven diffusive system with interactions between the particles is the following variant of the KLS model [6,18,21]. In the interior, particles at site i move to site $i+1$, provided it is empty, with a rate that depends on the state of sites $i-1$ and $i+2$:

$$0100 \to 0010 \text{ with rate } 1+\delta,$$

$$1100 \to 1010 \text{ with rate } 1+\epsilon,$$

$$0101 \to 0011 \text{ with rate } 1-\epsilon,$$

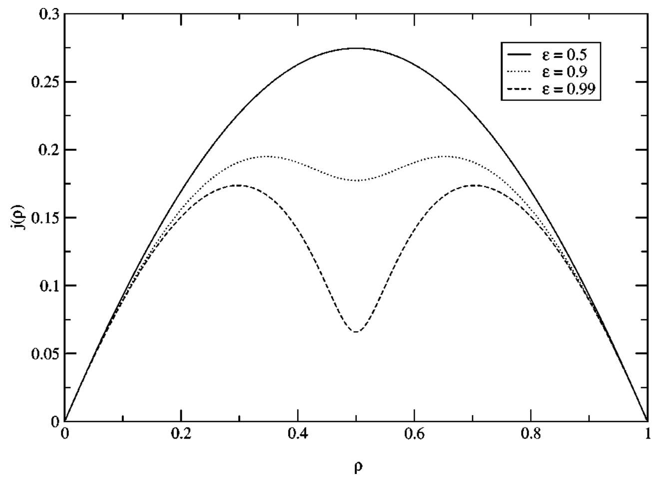

FIG. 3. Current-density relation for the one-dimensional KLS model for various ϵ.

$$1101 \rightarrow 1011 \quad \text{with rate} \quad 1-\delta.$$

At site 1, particles can enter the lattice provided the target site is empty. The rate depends on the state of site 2. Similarly, particles can leave the system at site L with a rate depending on the state of site $L-1$. The boundaries mimic the action of reservoirs with densities ρ_- and ρ_+. For $\rho_- = \rho_+$, the stationary state is that of an one-dimensional Ising model with boundary fields. The current-density relation can be calculated exactly using transfer matrix techniques [18]. It turns out that for strong enough repulsion between the particles ($\epsilon \gtrsim 0.9$), a current-density relation with two maxima arises (see Fig. 3). The parameter δ determines the skewness of $j(\rho)$ with respect to the vertical line $\rho = 1/2$. For $\delta = 0$, the system has particle-hole symmetry resulting in $j(\rho)$ being symmetric with respect to 1/2. For simplicity, we consider this case in the rest of the paper.

The phase diagram of this family of models with strong particle repulsion is known to exhibit seven different phases, among them are two maximal-current phases and one minimal-current phase. The phase diagram is determined by the interplay of diffusion, branching, and coalescence of shocks [21].

When equipping these models with Langmuir kinetics, one expects that a very rich phase diagram with many more than the original seven phases will appear. We will not attempt to give this full phase diagram here, but instead present two distinct features, which cannot be observed in systems without a concave region in the current-density relation: localized downward shocks and double shocks.

A. Localized downward shocks

In the regime where the current-density relation of the KLS model exhibits two maxima at densities ρ_1^* and ρ_2^*, where $\rho_1^* < \rho_2^*$ and a minimum at $\rho = 1/2$ (at $\delta = 0$), there is a region where downward shocks are stable according to Refs. [18,21] [and rule (c)]. These are characterized by $\rho_l \in (0.5, \rho_2^*)$ and $\rho_r \in (\rho_1^*, 0.5)$. This suggests that localized downwards shocks may appear when introducing the kinetic rates. Indeed, in the KLS model with Langmuir kinetics for certain values of the boundary densities ρ_- and ρ_+, which strongly depend on the kinetic rates Ω_a and Ω_b, one gets a stable downward shock according to rules (a)–(c). We give an example for this case in Fig. 4 (also refer to Fig. 5).

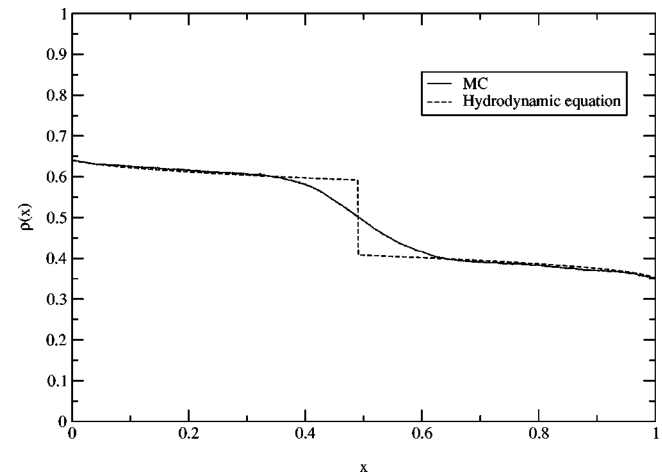

FIG. 4. Density of particles ρ versus rescaled coordinate x (*site number/L*) in a localized downward shock in the KLS model with Langmuir kinetics. Parameters are $\rho_- = 0.64$, $\rho_+ = 0.35$, and $\Omega_a = \Omega_d = 0.05$. We show the results of both hydrodynamic equation and Monte Carlo simulation for $L = 1000$. The smoothness of the MC result is due to the fluctuation of the shock position [16].

One can see that employing the general theory described above yields a stationary profile with a localized downward shock, which coincides with the MC results up to finite size effects, while a simple mean field approach would fail as it would not be able to capture the difference between the KLS model with $\epsilon > 0$ and the TASEP (KLS with $\epsilon = 0$).

B. Localized double shocks

Let $\rho'_{1,2}$ be defined as the inflection points of the current-density relation ($\rho'_1 < \rho'_2$). As is known from the studies of the KLS model [18,21], if we start an infinite system from a steplike initial density profile with $\rho_- \in (\tilde{\rho}_1, \rho'_1)$ on the left

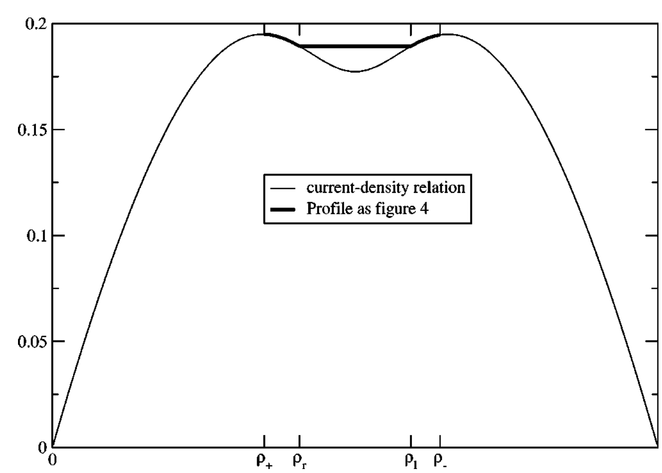

FIG. 5. Path in the current-density relation for the profile shown in Fig. 4.

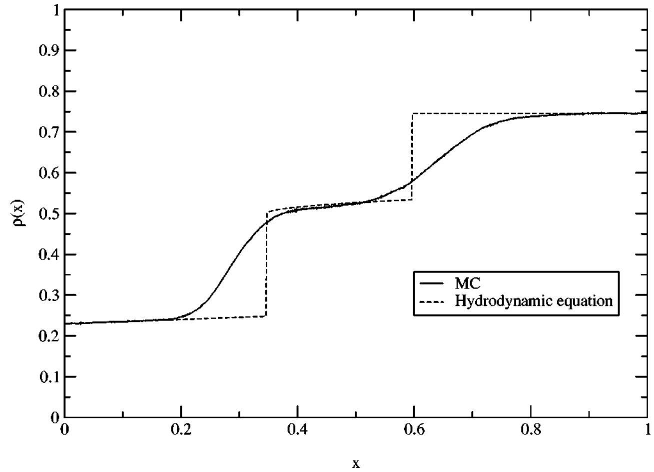

FIG. 6. Density of particles ρ versus rescaled coordinate x (*site number/L*) in a localized double shock in the KLS model with Langmuir kinetics. Parameters are $\rho_-=0.23$, $\rho_+=0.745$, $\Omega_a=0.03$, and $\Omega_d=0.01$. We show the results of both hydrodynamic equation and Monte Carlo simulation for $L=1000$. The smoothness of the MC result is due to the fluctuation of the shock position [16].

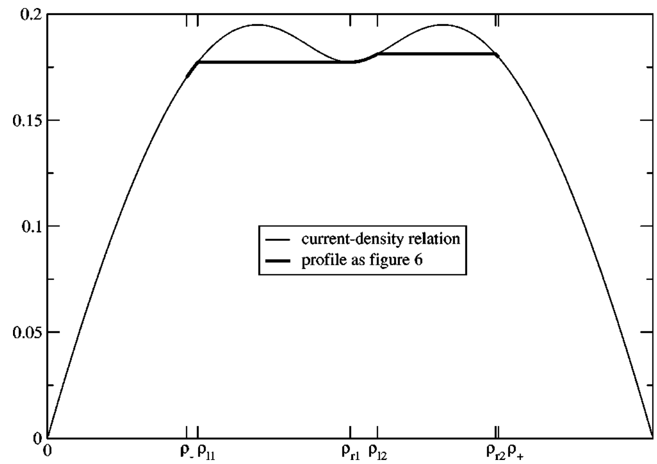

FIG. 7. Path in the current-density relation for the profile shown in Fig. 6.

and $\rho_+\in(\rho_2',\tilde{\rho}_2)$ on the right, we get a time-dependent solution having two shocks. One of these shocks has negative mean velocity, while the other has positive, and in the middle there is an expanding region with $\rho=1/2$ (for $\delta=0$) which corresponds to the minimal-current phase in a system with open boundaries [18,21].

This leads us to the conjecture that introducing the kinetic rates for certain values of ρ_-,ρ_+,Ω_a, and Ω_d, one may achieve a stable double shock structure. In Fig. 6 (see also Fig. 7), we present an example for such a case. Application of rules (a)–(c), which is presented in detail in the Appendix, yields the same double shock structure as the MC simulations up to finite size effects. Note, that a simple mean field approach could not predict a double shock.

V. CONCLUSIONS

In this work, we present a hydrodynamic equation which, together with some rules treating the discontinuities, correctly describes the stationary states of one-dimensional driven diffusive systems with Langmuir kinetics and open boundaries. It captures both systems without correlations in a steady state (as the TASEP and the k-hop exclusion models) and systems with correlations as the KLS model. For the latter, the two phenomena of a stationary localized downward shock and a localized double shock (corresponding to phase separation to three distinct regions) were presented, which a mean field approach would not reproduce. The exact current of driven diffusive systems without LK enters the hydrodynamic description since the bulk has sufficient time to relax between subsequent annihilation/creation events. An interesting paradoxical feature of these phenomena is that the fluctuating shocks get localized due to extra noise (LK), which is highly unexpected.

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APPENDIX: DOUBLE SHOCK DENSITY PROFILE FROM RULES (A)–(C)

Here, we demonstrate how one determines the stationary density profile using rules (a)–(c) from Sec. II. As an example, we take the parameters that yield a double

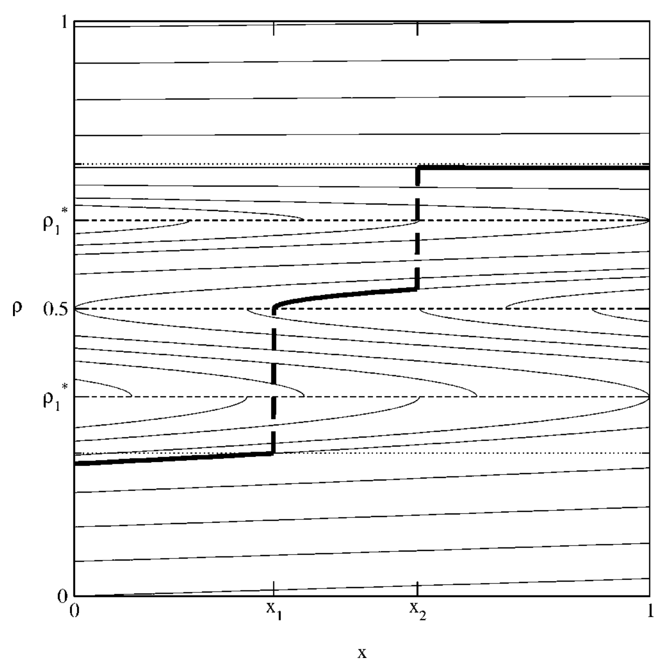

FIG. 8. The flow field of the hydrodynamic equation in the KLS model with Langmuir kinetics. Parameters are $\delta=0,\epsilon=0.9,\Omega_a=0.03$, and $\Omega_d=0.01$. The thick lines show the stationary density profile for $\rho_-=0.23,\rho_+=0.745$ given by rules (a)–(c). The dotted lines are $\rho=\tilde{\rho}_1\approx0.248\,21$, $\rho=\tilde{\rho}_2\approx0.751\,78$ (see Sec. IV B for notations). Axes: x is a rescaled coordinate (*site number/L*), $\rho(x)$ is an average density of particles at point x.

(localized) shock structure in the KLS model ($\rho_-=0.23$, $\rho_+=0.745$, $\Omega_a=0.03$, and $\Omega_d=0.01$). The KLS-model parameters are $\delta=0,\epsilon=0.9$ (see Sec. IV).

First assume that there is a boundary layer at $x=0$. According to rule (b), it is stable only if $\rho'_->1-\rho_-=0.77$. If this is the case then in the bulk there is no allowed jump since these trajectories of the flow field (see Fig. 8) stay always above $\rho=0.75$ [rules (a) and (c)], which yields $\rho'_+>0.75$. But then the boundary layer at $x=1$ does not satisfy rule (b). This contradiction shows that there is no boundary layer at $x=0$. One can use the same argument to show that there is no boundary layer at $x=1$ either.

Now one can see that the stationary density profile close to the left boundary follows the line of the flow field for which $\rho(x=0)=\rho_-=0.23$. Since there is no boundary layer at the right end, it is clear that somewhere in the bulk it has to make a jump.

Note that this trajectory crosses the line $\rho=\tilde{\rho}_1$ at $x=x_1$. Suppose that the jump takes place before at $x<x_1$. In this case, according to rule (a), it would jump over $\tilde{\rho}_2=1-\tilde{\rho}_1$ which would result in a boundary layer at $x=1$, which is not allowed. If the jump takes place at $x>x_1$, then $\rho_1^*<\rho_r<0.5$ and since from this region there is no allowed jump it would end up at $\rho_1^*<\rho'_+<0.5$, resulting again in an unstable boundary layer on the right side. This shows that the jump is located at $x=x_1$, and from here the density profile follows the trajectory that starts at $x=x_1$ with the value $\rho=0.5+0$.

One can easily see that we need another jump to connect this trajectory with the one that ends at $x=1$ with $\rho=\rho_+$. Applying rule (a) (continuity of the current), we can get the point x_2 where the second jump is located.

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