

Exact Shock Measures and Steady-State Selection in a Driven Diffusive System with Two Conserved Densities

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We study driven 1d lattice gas models with two types of particles and nearest neighbor hopping. We find the most general case when there is a shock solution with a product measure which has a density-profile of a step function for both densities. The position of the shock performs a biased random walk. We calculate the microscopic hopping rates of the shock. We also construct the hydrodynamic limit of the model and solve the resulting hyperbolic system of conservation laws. In case of open boundaries the selected steady state is given in terms of the boundary densities.

KEY WORDS: Two-species ASEP; hydrodynamic limit; shock measure; systems of conservation laws; steady-state selection.

1. INTRODUCTION

On the macroscopic level driven diffusive systems are often described by hydrodynamic equations for some relevant parameters (usually the particle densities). These partial differential equations are generally nonlinear and can develop shocks, i.e., discontinuities in the space dependence of the densities. These shocks behave as collective excitations in systems with one conservation law: they can be characterized by only one parameter, namely their position, and the propagation can be described by single particle dynamics.

Recently much attention was paid to the investigation of the stationary microscopic structure^(1–3) and the microscopic dynamics^(4–8) of such shocks. Mostly the well-known asymmetric simple exclusion process (ASEP) was studied: it was pointed out in ref. 7 (and for infinite systems

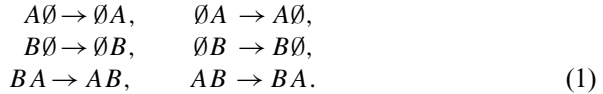
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in ref. 6) that for special tuning of densities and microscopic hopping rates there exists a travelling shock with a step-like density profile even on the microscopic scale, which behaves like a collective one-particle excitation. However, little is known about the microscopic structure and dynamics of shocks in systems with two conservation laws,^(9–12) which recently have become a focus of attention (for a review see ref. 13 and ref. 14, 15 for more recent work).

In the present work we show that a shock measure with single-particle dynamics can describe also systems with two conserved densities, introduced in Section 2. The position of the shock performs a biased random walk just like in the ASEP (Section 3). In Section 4 we study the hydrodynamic limit of the model (under Eulerian scaling) which shows a larger class of stable shock solutions. The hierarchical structure of the hydrodynamic equations for this system allows us to deduct the steady state selection in an open system connected to particle reservoirs at its boundaries.

2. TWO-SPECIES EXCLUSION PROCESS

The model is defined on an open lattice with L sites and two types of particles (A and B). Each lattice site can either be occupied by a particle, which can be either A or B , or can be vacant (\emptyset). Having two independent conserved quantities requires that only hopping processes are allowed. For simplicity we allow just for nearest neighbour hoppings. These are the following:



A state of the model is defined through a probability measure P_η on the set of all configurations $\eta = (\eta_1, \eta_2, \dots, \eta_L)$, $\eta_k \in \{A, B, \emptyset\}$. For our purposes it is convenient to use the Hamiltonian formalism⁽¹⁶⁾ where one assigns a basis vector $|\eta\rangle$ of the vector space $(\mathbb{C}^3)^{\otimes L}$ to each configuration and the probability vector is defined by $|P\rangle = \sum_\eta P_\eta |\eta\rangle$. It is normalized such that $\langle s|P\rangle = 1$, where $\langle s| = \sum_\eta \langle \eta|$. The time dependence is now described by the master equation

$$\frac{d}{dt} |P(t)\rangle = -H |P(t)\rangle,
 \tag{2}$$

through a ‘‘Hamiltonian’’ H which has as matrix elements $H_{\eta,\eta'}$ the hopping rates between configurations η, η' . Since we have only nearest-neighbor exchange processes the Hamiltonian in (2) can be written as

$$H = h_1 + \sum_{k=1}^{L-1} h_{k,k+1} + h_L, \quad (3)$$

where $h_{k,k+1}$ acts nontrivially only on sites k and $k+1$ (corresponding to hopping) while h_1, h_L generates boundary processes specified below. Let $W_{\theta'_1\theta'_2}^{\theta_1\theta_2}$ ($\theta_1, \theta_2, \theta'_1, \theta'_2 \in \{A, B, \emptyset\}$) be an operator on $\mathbb{C}^3 \otimes \mathbb{C}^3$ which acts on the basis vectors $|\eta_1, \eta_2\rangle$ as

$$W_{\theta'_1\theta'_2}^{\theta_1\theta_2} |\eta_1, \eta_2\rangle = \delta_{\eta_1\theta_1} \delta_{\eta_2\theta_2} |\theta'_1, \theta'_2\rangle. \quad (4)$$

Then $h_{k,k+1}$ can be written as

$$h_{k,k+1} = \mathbb{1}^{\otimes(k-1)} \otimes \left[\sum_{\theta_1\theta_2\theta'_1\theta'_2} -\Gamma_{\theta'_1\theta'_2}^{\theta_1\theta_2} \left(W_{\theta'_1\theta'_2}^{\theta_1\theta_2} - W_{\theta_1\theta_2}^{\theta'_1\theta'_2} \right) \right] \otimes \mathbb{1}^{\otimes(L-k-1)}. \quad (5)$$

The diagonal term in (5) stands for the conservation of probability. The model is defined through the rates $\Gamma_{\theta'_1\theta'_2}^{\theta_1\theta_2}$ which describe the hopping process $\theta_1\theta_2 \rightarrow \theta'_1\theta'_2$. In our model the nonzero rates are the following:

$$\begin{aligned} \Gamma_{\emptyset A}^{A\emptyset} &= a_1, & \Gamma_{A\emptyset}^{\emptyset A} &= a_2, \\ \Gamma_{\emptyset B}^{B\emptyset} &= b_1, & \Gamma_{B\emptyset}^{\emptyset B} &= b_2, \\ \Gamma_{AB}^{BA} &= c_1, & \Gamma_{BA}^{AB} &= c_2. \end{aligned}$$

The boundary terms h_1 and h_L in (3) act only on the first and L th site, respectively and choosing the basis

$$|A\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |B\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad |\emptyset\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad (6)$$

they have the form

$$h_1 = \begin{pmatrix} \beta_l^A + \gamma_l^- & -\alpha_l^A & -\gamma_l^+ \\ -\beta_l^A & \alpha_l^A + \alpha_l^B & -\beta_l^B \\ -\gamma_l^- & -\alpha_l^B & \beta_l^B + \gamma_l^+ \end{pmatrix} \otimes \mathbb{1}^{\otimes(L-1)}, \quad (7)$$

$$h_L = \mathbb{1}^{\otimes(L-1)} \otimes \begin{pmatrix} \beta_r^A + \gamma_r^- & -\alpha_r^A & -\gamma_r^+ \\ -\beta_r^A & \alpha_r^A + \alpha_r^B & -\beta_r^B \\ -\gamma_r^- & -\alpha_r^B & \beta_r^B + \gamma_r^+ \end{pmatrix}, \quad (8)$$

where $\alpha^{A(B)}$, $\beta^{A(B)}$ and $\gamma^{+(-)}$ are the rates for the following processes:

$$\alpha^A : \emptyset \rightarrow A, \quad \alpha^B : \emptyset \rightarrow B, \quad (9)$$

$$\beta^A : A \rightarrow \emptyset, \quad \beta^B : B \rightarrow \emptyset, \quad (10)$$

$$\gamma^+ : B \rightarrow A, \quad \gamma^- : A \rightarrow B, \quad (11)$$

and the indexes l and r indicate the left and right boundary, respectively.

It is known that in the finite periodic system there is a family of steady states which are product measures.^(11,17) We call P_η a product measure if it has the form

$$P_\eta = P_{\eta_1}^{(1)} P_{\eta_2}^{(2)} \dots P_{\eta_L}^{(L)}, \quad (12)$$

where $P_{\eta_k}^{(k)}$ is a probability measure on $\{A, B, \emptyset\}$. This means that the probability vector has the following direct product form

$$\begin{aligned} |P\rangle &= \begin{pmatrix} p_1^A \\ 1 - p_1^A - p_1^B \\ p_1^B \end{pmatrix} \otimes \begin{pmatrix} p_2^A \\ 1 - p_2^A - p_2^B \\ p_2^B \end{pmatrix} \\ &\otimes \dots \otimes \begin{pmatrix} p_L^A \\ 1 - p_L^A - p_L^B \\ p_L^B \end{pmatrix}, \end{aligned} \quad (13)$$

where p_k^X is the probability of finding an “ X ” particle on site k .

Straightforward calculations show that for having a stationary product measure with uniform densities

$$|P\rangle = \left(\begin{pmatrix} \rho^A \\ 1 - \rho^A - \rho^B \\ \rho^B \end{pmatrix} \right)^{\otimes L}, \quad (14)$$

the rates have to satisfy the following condition^(11,17)

$$a_1 - a_2 - b_1 + b_2 + c_1 - c_2 = 0. \quad (15)$$

This is already a sufficient condition in case of an infinite chain or periodic boundary conditions. For open boundaries there are some additional restrictions for the boundary rates, for which we find

$$\begin{aligned} & (a_1 - a_2)\rho^A(1 - \rho^A) - (b_1 - b_2)\rho^A\rho^B \\ & = \alpha_l^A(1 - \rho^A - \rho^B) - (\beta_l^A + \gamma_l^-)\rho^A + \gamma_l^+\rho^B \end{aligned} \quad (16)$$

$$= (\beta_r^A + \gamma_r^-)\rho^A - \alpha_r^A(1 - \rho^A - \rho^B) - \gamma_r^+\rho^B, \quad (17)$$

$$\begin{aligned} & (b_1 - b_2)\rho^B(1 - \rho^B) - (a_1 - a_2)\rho^A\rho^B \\ & = \alpha_l^B(1 - \rho^A - \rho^B) - (\beta_l^B + \gamma_l^+)\rho^B + \gamma_l^-\rho^A \end{aligned} \quad (18)$$

$$= (\beta_r^B + \gamma_r^+)\rho^B - \alpha_r^B(1 - \rho^A - \rho^B) - \gamma_r^-\rho^A. \quad (19)$$

The physical meaning of these equations is that the steady state currents of the conserved densities have to be fitted at the boundaries. In the following we will assume that condition (15) is fulfilled. For boundary rates as given above we say that the system is in contact with a reservoir of densities $\rho^{A,B}$.

3. TIME-DEPENDENT SHOCK MEASURES

Krebs *et al.* in ref. 7 pointed out that in the ASEP with open boundaries there is a family of shock measures which closes under the time evolution of the process, i.e., an initial measure from this family evolves into a linear combination of measures from this family. Below we shall refer to such a set as an invariant family of shock measures. Each element is a product measure with a step-like density profile; $\rho_{l(r)}$ on the left (right) of the shock. These shock measures are characterised by the position of the shock. If $|P_k\rangle$ is a state having the shock between the sites k and $k+1$ then these states for $k=0, 1, 2, \dots, L$ generate a subspace of the vector-space of states which is invariant under time evolution and thus the many-particle problem is reduced to a one-particle one. This property holds if the densities $\rho_{l,r}$ satisfy the condition

$$\frac{p}{q} = \frac{\rho_r(1 - \rho_l)}{\rho_l(1 - \rho_r)}, \quad (20)$$

where p and q are the hopping rates of the particles to the right resp. left. The resulting one-particle dynamics have a natural interpretation as a simple random walk of the shock position (see Fig. 1).

In the following we search for the conditions under which there exists in our three-state model an invariant family of shock measures which are

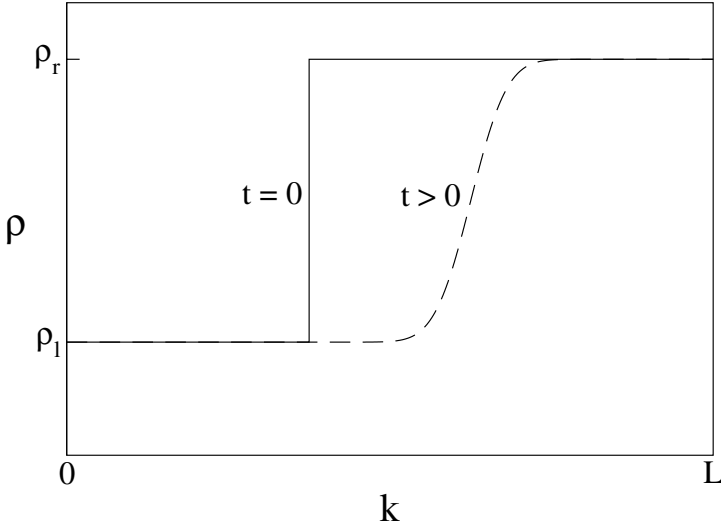


Fig. 1. Time dependence of the density profile in the one-species ASEP starting from a shock measure satisfying (20). For positive times the measure is a diffusive linear combination of step-like shock measures.

product measures with a jump in the local particle density. To this end let $|P_k\rangle$ be defined as

$$|P_k\rangle = \begin{pmatrix} \rho_l^A & \\ 1 - \rho_l^A - \rho_l^B & \\ \rho_l^B & \end{pmatrix}^{\otimes k} \otimes \begin{pmatrix} \rho_r^A & \\ 1 - \rho_r^A - \rho_r^B & \\ \rho_r^B & \end{pmatrix}^{\otimes L-k}. \quad (21)$$

The probability vectors $|P_k\rangle$ define an $L + 1$ -dimensional subspace of the vector space on which H acts. Closure of this family of shock measures under the time evolution generated by H is equivalent to requiring

$$H|P_k\rangle = -d_r|P_{k+1}\rangle - d_l|P_{k-1}\rangle + (d_r + d_l)|P_k\rangle \quad (22)$$

for $1 \leq k \leq L - 1$, and

$$H|P_0\rangle = -\bar{d}_r|P_1\rangle + \bar{d}_r|P_0\rangle, \quad (23)$$

$$H|P_L\rangle = -\bar{d}_l|P_{L-1}\rangle + \bar{d}_l|P_L\rangle. \quad (24)$$

This is easy to see because of having only nearest neighbour interactions double hoppings of the shock position (e.g. $|P_k\rangle \rightarrow |P_{k+2}\rangle$) cannot occur. If

this condition can be met by an appropriate choice of model parameters the quantities $d_{l,r}$ and $\tilde{d}_{l,r}$ are non-negative real numbers representing the hopping rates of the shock in the bulk ($d_{l,r}$) and at the boundaries ($\tilde{d}_{l,r}$).

To investigate whether (22–24) can be satisfied it is better to rewrite the Hamiltonian in the form

$$H = h_1 + (a_1 - a_2)n_1^A + (b_1 - b_2)n_1^B + \sum_{k=1}^{L-1} \tilde{h}_{k,k+1} + h_L - (a_1 - a_2)n_L^A - (b_1 - b_2)n_L^B, \quad (25)$$

where

$$\tilde{h}_{k,k+1} = h_{k,k+1} - (a_1 - a_2)(n_k^A - n_{k+1}^A) - (b_1 - b_2)(n_k^B - n_{k+1}^B). \quad (26)$$

Here and in (25) n_k^A and n_k^B are the particle number operators for the A and B particles on site k .

As a result $\tilde{h}_{k,k+1}|P_l\rangle = 0$ for $k \neq l$. Therefore, one has

$$H|P_k\rangle = \tilde{h}_{k,k+1}|P_k\rangle + \left(h_1 + h_L + (a_1 - a_2)(n_1^A - n_L^A) + (b_1 - b_2)(n_1^B - n_L^B) \right) |P_k\rangle \quad (27)$$

for $1 \leq k \leq L-1$, and

$$H|P_k\rangle = \left(h_1 + h_L + (a_1 - a_2)(n_1^A - n_L^A) + (b_1 - b_2)(n_1^B - n_L^B) \right) |P_k\rangle \quad (28)$$

for $k=0, L$.

At the boundaries one has to satisfy (16) with the slight modification that on the left (right) boundary we write $\rho_l^{A,B}$ ($\rho_r^{A,B}$) instead of $\rho^{A,B}$

$$\alpha_l^A(1 - \rho_l^A - \rho_l^B) - (\beta_l^A + \gamma_l^-)\rho_l^A + \gamma_l^+\rho_l^B = (a_1 - a_2)\rho_l^A(1 - \rho_l^A) - (b_1 - b_2)\rho_l^A\rho_l^B, \quad (29)$$

$$(\beta_r^A + \gamma_r^-)\rho_r^A - \gamma_r^+\rho_r^B - \alpha_r^A(1 - \rho_r^A - \rho_r^B) = (a_1 - a_2)\rho_r^A(1 - \rho_r^A) - (b_1 - b_2)\rho_r^A\rho_r^B, \quad (30)$$

and the same for the B particles

$$\begin{aligned} & \alpha_l^B (1 - \rho_l^A - \rho_l^B) - (\beta_l^B + \gamma_l^+) \rho_l^B + \gamma_l^- \rho_l^A \\ & = (b_1 - b_2) \rho_l^B (1 - \rho_l^B) - (a_1 - a_2) \rho_l^A \rho_l^B, \end{aligned} \quad (31)$$

$$\begin{aligned} & (\beta_r^B + \gamma_r^+) \rho_r^B - \gamma_r^- \rho_r^A - \alpha_r^B (1 - \rho_r^A - \rho_r^B) \\ & = (b_1 - b_2) \rho_r^B (1 - \rho_r^B) - (a_1 - a_2) \rho_r^A \rho_r^B. \end{aligned} \quad (32)$$

This fixes a manifold of boundary parameters required to satisfy (22–24). The physical interpretation is a connection to boundary reservoirs with different left and right densities respectively. Requiring (29–32) for the boundary operators h_1 and h_L simplifies (27) and leads to

$$\begin{aligned} H|P_k\rangle &= \tilde{h}_{k,k+1}|P_k\rangle \\ &+ \left((a_1 - a_2)(\rho_l^A - \rho_r^A) \right. \\ &+ \left. (b_1 - b_2)(\rho_l^B - \rho_r^B) \right) |P_k\rangle \end{aligned} \quad (33)$$

for $1 \leq k \leq L - 1$. Thus satisfying (22) is equivalent to requiring

$$\begin{aligned} \tilde{h}_{k,k+1}|P_k\rangle &= -d_r|P_{k+1}\rangle - d_l|P_{k-1}\rangle \\ &+ \left(d_r + d_l - (a_1 - a_2)(\rho_l^A - \rho_r^A) \right. \\ &- \left. (b_1 - b_2)(\rho_l^B - \rho_r^B) \right) |P_k\rangle \end{aligned} \quad (34)$$

for $1 \leq k \leq L - 1$. Straightforward but lengthy calculation shows that $\tilde{h}_{k,k+1}|P_k\rangle$ has this form for $1 \leq k \leq L - 1$ if and only if

$$a_1 = b_1 =: p, \quad a_2 = b_2 =: q, \quad (35)$$

$$\frac{p}{q} = \frac{\rho_r(1 - \rho_l)}{\rho_l(1 - \rho_r)}, \quad (36)$$

$$\frac{\rho_l^A}{\rho_l^B} = \frac{\rho_r^A}{\rho_r^B} =: r, \quad (37)$$

where $\rho_{l(r)} = \rho_{l(r)}^A + \rho_{l(r)}^B$ is the total density of particles on the left (right) of the shock. We note here that (35) together with (15) gives also $c_1 = c_2$. This means that the A and B particles behave the same way: the hopping rates to the left and to the right are p and q for both and also the exchange rates c_1 and c_2 are the same in both directions. Equations (23,24) give extra conditions for the boundary rates, namely

$$\alpha_l^A = r\alpha_l^B \quad \alpha_r^A = r\alpha_r^B. \quad (38)$$

This together with (29–32) give conditions also for the boundary rates $\beta_{l,r}^{A,B}$ and $\gamma_{l,r}^{+-}$.

The rates d_r and d_l which describe the diffusion of the shock position to the right and to the left are

$$d_r = \frac{\rho_r}{\rho_l} q = \frac{1 - \rho_r}{1 - \rho_l} p, \quad d_l = \frac{\rho_l}{\rho_r} p = \frac{1 - \rho_l}{1 - \rho_r} q. \quad (39)$$

In addition we find the boundary rates

$$\begin{aligned} \bar{d}_r &= \frac{\alpha_l}{\rho_l} - \rho_r(p - q) = (p - q)(1 - \rho_r) \\ &\quad + \frac{r\beta_l^A + \beta_l^B}{(r + 1)(1 - \rho_l)}, \end{aligned} \quad (40)$$

$$\begin{aligned} \bar{d}_l &= \frac{\alpha_r}{\rho_r} + \rho_l(p - q) = -(p - q)(1 - \rho_l) \\ &\quad + \frac{r\beta_r^A + \beta_r^B}{(r + 1)(1 - \rho_r)}, \end{aligned} \quad (41)$$

where $\alpha_{l(r)} = \alpha_{l(r)}^A + \alpha_{l(r)}^B$.

Using (36) the bulk shock hopping rates (39) become

$$d_{l(r)} = (p - q) \frac{\rho_{l(r)}(1 - \rho_{l(r)})}{\rho_r - \rho_l} \quad (42)$$

as in the ASEP.^(6,7) Since by identifying A and B particles one arrives at the one-species ASEP, it is not surprising that (36) and (42) are in full agreement with the corresponding formulas of the ASEP. The novelty is that (a) the family of product measures with step-like density profiles satisfying (37) remains invariant even if one distinguishes between A and B particles, (b) there is no other possibility for having such an invariant family of shock measures (up to relabelling the states A, B and \emptyset). Notice that this solution describes a *single* shock whereas generically a system with two conservation is expected to have two stationary shocks.^(9,12)

4. HYDRODYNAMIC LIMIT

4.1. Derivation of the Partial Differential Equation

In the previous sections the microscopic dynamics of the two-species ASEP was studied. It was found that there is an invariant family of product measures with step-like density profiles if criterion (35) for the rates

and criteria (36), (37) for the densities are fulfilled. It is also of interest to drop the conditions (36), (37) and see how this model behaves on the macroscopic scale, i.e., when the space and time is rescaled as $t_{\text{mac}} = t_{\text{mic}} a$, $x = ka$ and the lattice spacing $a \rightarrow 0$ (Eulerian scaling). In this subsection we restrict the discussion to the case of infinite chains (or torus geometry). Finite systems with open boundaries are considered in the last subsection.

Performing the Euler scaling one can easily construct the naive hydrodynamic equations of a model having two conserved quantities (v and u) and stationary product measure. These describe the macroscopic time-evolution of the conserved quantities

$$\partial_t v + \partial_x j_v(v, u) = 0, \quad (43)$$

$$\partial_t u + \partial_x j_u(v, u) = 0, \quad (44)$$

where $j_v(v, u)$ and $j_u(v, u)$ are the currents of v and u assuming homogeneous product measure. It is important to note that the hydrodynamic limit of a driven lattice gas is different from the continuum mean-field description: while both of them deals only with averages the latter neglects the local correlations while the former does not. Our case is exceptional in the sense that the *exact* currents as a function of the densities—which one has to know for the correct hydrodynamic limit—are the same as the mean-field currents. This is due to the fact that in our system the homogeneous product measure is stationary (15). In other systems, where this does not hold, the naive mean-field description (even improved mean-field approaches) would usually fail in the continuum limit even if there are only short range correlations. We also have to note that even in case of product measure stationary states it is far from trivial that the above set of conservation laws describe correctly the macroscopic dynamics of the model. However, a mathematically rigorous proof is available that in all systems having nearest neighbor dynamics with two conserved densities (v and u) and stationary product measure, the time evolution of the densities under Eulerian scaling is described by Eqs. (43) and (44) until the occurrence of the first shock.⁽¹¹⁾ For closely related results on two-species systems, see refs. 12,14, for an apparent failure of the hydrodynamic description, see ref. 15 and earlier work on condensation in two-species systems.^(13,18,19)

For our model it is useful to introduce the new set of conserved quantities (v, u) instead of (ρ^A, ρ^B)

$$v = 1 - \rho^A - \rho^B \quad (\text{the density of vacancies}), \quad (45)$$

$$u = \rho^A - \rho^B. \quad (46)$$

The associated currents are

$$j_v = -(p - q)v(1 - v), \quad (47)$$

$$j_u = (p - q)vu. \quad (48)$$

Plugging these into (43) and (44) one arrives to the hydrodynamic equations of the model

$$\partial_t v - (p - q)\partial_x(v(1 - v)) = 0, \quad (49)$$

$$\partial_t u + (p - q)\partial_x(vu) = 0. \quad (50)$$

In the special case when $p = q$ the currents are zero and the solution of (43) and (44) becomes trivial. In this case the behaviour of the microscopic model is diffusive so one has to perform diffusive scaling ($t_{\text{mac}} = t_{\text{mic}}a^2$, $x = ka$, $a \rightarrow 0$) to see the nontrivial macroscopic behaviour.

It is to be noted that the generic set of PDEs describing systems with three local states and satisfying (15) is the so-called Leroux's system:^(11,12)

$$\partial_t \sigma + \partial_x(\sigma \tau) = 0, \quad (51)$$

$$\partial_t \tau + \partial_x(\sigma + \tau^2) = 0. \quad (52)$$

It means that there are always such linear combinations (σ, τ) of the conserved quantities (shifted by an irrelevant constant) which satisfy (51) and (52).⁽¹¹⁾ However, in our case, when $a_1 = b_1$ and $a_2 = b_2$, σ and τ turn out to be linearly dependent and Eq. (51) and (52) are equivalent (and correspond to (49)). Therefore our model has to be investigated separately.

Note that Eq. (49) for v is decoupled from u and takes the form of the well-known Burgers equation, which can be solved exactly⁽²⁰⁾. Introducing

$$\phi = (\rho^A - \rho^B)/(\rho^A + \rho^B) = u/(1 - v), \quad (53)$$

one gets the linear wave equation for ϕ

$$\partial_t \phi + (p - q)v\partial_x \phi = 0, \quad (54)$$

meaning that ϕ is constant along the curves $x(t)$ satisfying the ordinary differential equation

$$\frac{dx}{dt} = v(x, t), \quad (55)$$

where $v(x, t)$ is the solution of (49). The physical meaning of $x(t)$ is that this is the expected path of a single tagged particle (either A or B).

4.2. Development of an Initial Sharp Interface

Suppose that at $t=0$ there is a sharp interface separating domains characterised by $v_{l(r)}$ and $u_{l(r)}$ on the left (right), respectively. We assume that $v_l > v_r$ in order to guarantee the stability of the interface.^(9,16) No further conditions on the values of u, v are imposed.

The time and space dependence of v is known since it is described by the inviscid Burgers equation (49): the step-like front (having $v_{l(r)}$ on the left (right) of it) is travelling with velocity

$$V_1 = (q - p)(1 - v_l - v_r). \quad (56)$$

The $x(t)$ curves defined by equation (55) are then broken lines as in Fig. 2. One can see that ϕ changes while crossing the dashed line indicating that there is another shock in the system travelling with larger velocity (without loss of generality we assume that $p > q$)

$$V_2 = (p - q)v_r > V_1. \quad (57)$$

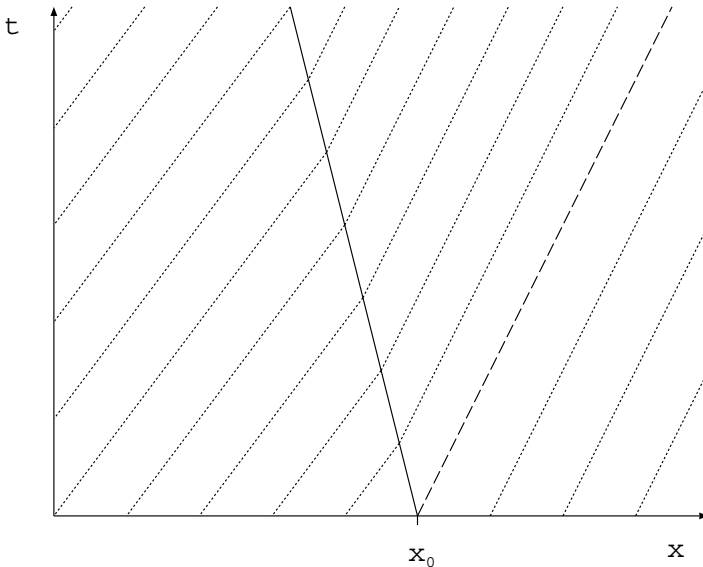


Fig. 2. The $x(t)$ curves of equation (55) for the case when $v(x, t)$ is a shock-solution of the Burgers equation (49). The position of this shock (starting from x_0) is marked by the thick solid line. u also changes on the dashed line indicating another shock in the system, but this is not microscopically sharp.

Generally a single sharp interface at $t=0$ forms two shocks (or rarefaction waves) at $t>0$ in systems having two conservation laws.⁽⁹⁾ For the complete analysis one has to study the eigenvalues and eigenvectors of the Jacobian

$$\frac{\partial(j_u, j_v)}{\partial(u, v)} = (p-q) \begin{pmatrix} v & u \\ 0 & 2v-1 \end{pmatrix}, \quad (58)$$

which give the characteristic velocities of the different types of density fluctuations.⁽⁹⁾ In this specific system these are

$$\lambda_1 = (p-q)(2v-1), \quad e_1 = \begin{pmatrix} u \\ v-1 \end{pmatrix}, \quad (59)$$

$$\lambda_2 = (p-q)v, \quad e_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (60)$$

The two corresponding types of shocks have either constant ϕ across the discontinuity (type 1, occurring along the solid line in Fig. 2) or constant v (type 2, occurring along the dashed line in Fig. 2). A shock (microscopically sharp interface) satisfying either of these relations initially does not split, whereas a generic shock splits into two shocks of type 1 and type 2 respectively. We remark that condition (37) translates into $\phi_l = \phi_r$ for the quantity ϕ . Hence the shock studied in the previous section is of type 1. Notice also that in the second mode u is changed but v is not. Walking along these lines in the (u, v) space λ_1 remains unchanged. This means that if there is a discontinuity in u (with constant v) then the fluctuations in u are not driven towards the “shock” but they travel with the same mean velocity resulting in an unstable shock on the microscopic scale. However, since in the original lattice model the width of the step is expected to scale with \sqrt{t} due to the diffusive dynamics of A and B particles the interface remains sharp under Eulerian scaling.

The physical significance of two types of shocks can be easily demonstrated considering the following example: at $t=0$ the system is partially occupied with only A particles on the left of x_0 and fully occupied by B particles on the right. This setting models a situation where particles (A) fall down (e.g. due to gravity) and enter a medium (B) where they have no weight. Hence they penetrate diffusively (with vanishing macroscopic flux), but pile up ballistically due to the constant incoming macroscopic flux. As a result two interfaces emerge (see Fig. 3). The second (lower) interface has velocity 0 since $v_r=0$, see (57). Although the particles diffuse and start mixing on the lattice scale at the A – B interface, this remains invisible on the Euler scale.

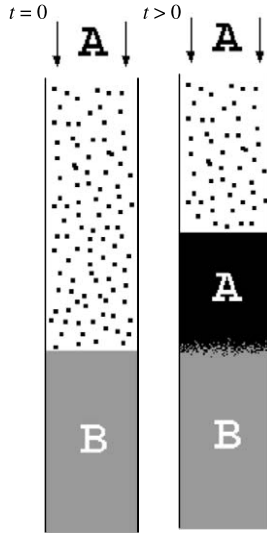


Fig. 3. The time development from a special initial condition: A particles fall down (e.g. due to gravity) and enter a medium where they have no weight, hence they penetrate diffusively but pile up ballistically resulting in two interfaces. The width of the domain wall between the A (black) and B (gray) particles scales with \sqrt{t} while the other domain wall remains microscopically sharp (however, on a diffusive scale one could see the fluctuations of the position of this sharp interface).

The other interface (type 1) separating domains with different densities of A particles corresponds to the usual shocks which are known from the study of the Burgers equation. Here both u and v are changed (but ϕ remains constant).

In Fig. 4 we show a more general example for the time development of the system starting from an initial state having a step in both densities at the origin. The second mode also can develop rarefaction waves if the density on the left is lower than on the right in the initial state. We note that the shock coming from the second mode always stays to the right of the shock/rarefaction wave coming from the first mode since it is faster (57).

4.3. Steady-State Selection in the Open System

In a finite system with open boundaries one is left with the question of steady state selection. In the infinite system all the states with constant density profiles are stationary, however, in the finite system with bound-

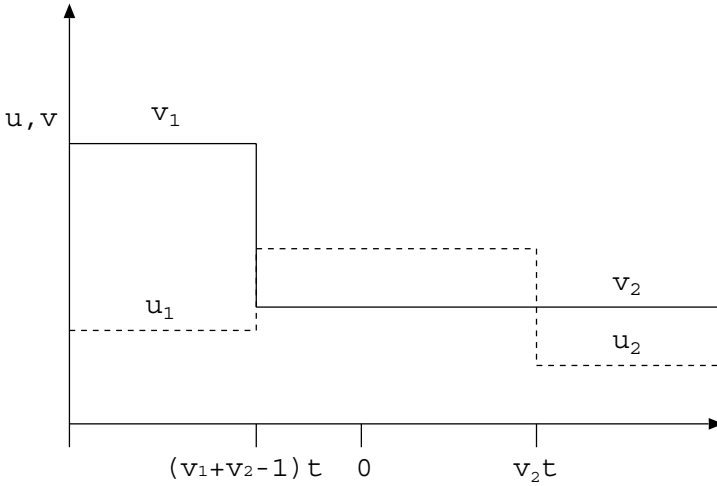


Fig. 4. Development of the densities v and u under Eulerian scaling starting from an initial state with step-like density profiles: v_1, u_1 on the left and v_2, u_2 on the right of the origin. The first interface (on the left) is a shock coming from the Burgers-equation and corresponds to the solid line in Fig. 2. The second one (on the right) is not microscopically sharp. In Fig. 2 it is the dashed line.

aries acting as particle reservoirs the bulk densities depend non-trivially on the boundary densities. Setting $\partial_t = 0$ in (43) and (44) one arrives at the solution that u and v are constant, so in general the densities cannot fit both boundaries. This discrepancy is resolved by the appearance of shocks in the original lattice model leading to discontinuities at either (or both) boundary in the hydrodynamic limit.

In case of one conserved density the density-current relation already determines the phase diagram in terms of the boundary densities^(21,22) but in case of more conservation laws the question turns out to be much more intricate and no general rule is known to apply.⁽¹⁰⁾ However, in our model it is possible to determine the resulting steady state for given boundary densities.

Since the dynamics of v is independent of u and follows the usual ASEP dynamics the profile can be deduced from the ASEP phase diagram.^(23–25) Our task is then to determine the bulk value of u in terms of the boundary densities $u_{\text{left}}, u_{\text{right}}, v_{\text{left}}, v_{\text{right}}$.

Since all the fluctuations in u travel with velocity $v \geq 0$ one would think that u_{bulk} is only determined by the left boundary if $v \neq 0$. However, this is not the case because a discontinuity in v can be localised at this boundary which also induce a step in u . The previously introduced

ϕ , however, does not change at this discontinuity which suggests that the bulk value of ϕ is given by the left boundary ($\phi_{\text{bulk}} = \phi_{\text{left}}$). In order to verify this heuristic reasoning we make use of a technique to determine the steady state which is widely used for systems with a single conservation law. One introduces a viscosity term in (43) and (44) proportional to ν which contain a second derivative of the densities leading to second order equations for the stationary profiles. Now the profiles can fit both boundaries for any value of ν and after performing limit $\nu \rightarrow 0$ one can get the selected density.

In case of one single conservation law this technique is quite robust in the sense that the resulting bulk density is essentially independent of the specific choice of the viscosity term (as long as it contains a second order derivative). For more conservation laws this method is mathematically not well-studied and one has to be more careful with the choice of viscosity term. For systems with a stationary product measure there is a natural choice for these terms introduced in ref. 9. Namely, when one derives the hydrodynamic equations from the lattice continuity equations one uses a Taylor expansion of the current (as a function of the densities) in the lattice constant. Keeping the second order terms leads to a unique viscosity term which is proportional to the lattice constant a .

In Appendix A we show that using this technique for our model the above conjecture, that $\phi_{\text{bulk}} = \phi_{\text{left}}$, is confirmed if $v_{\text{right}} \neq 0$, which implies

$$u = u_{\text{left}} \frac{1 - v}{1 - v_{\text{left}}} \quad \text{if } v_{\text{right}} \neq 0. \quad (61)$$

Summarizing the results (see also Fig. 5) we find

$$v_{\text{bulk}} = \begin{cases} v_{\text{left}} & \text{if } v_{\text{left}} \geq 1/2 \quad \text{and} \quad v_{\text{right}} > 1 - v_{\text{left}}, \\ v_{\text{right}} & \text{if } v_{\text{right}} \leq 1/2 \quad \text{and} \quad v_{\text{right}} < 1 - v_{\text{left}}, \\ 1/2 & \text{if } v_{\text{left}} \leq 1/2 \quad \text{and} \quad v_{\text{right}} \geq 1/2, \end{cases} \quad (62)$$

$$u_{\text{bulk}} = u_{\text{left}} \frac{1 - v_{\text{bulk}}}{1 - v_{\text{left}}} = \begin{cases} u_{\text{left}} & \text{if } v_{\text{left}} \geq 1/2 \quad \text{and} \quad v_{\text{right}} > 1 - v_{\text{left}}, \\ u_{\text{left}} \frac{1 - v_{\text{right}}}{1 - v_{\text{left}}} & \text{if } 0 < v_{\text{right}} \leq 1/2 \quad \text{and} \quad v_{\text{right}} < 1 - v_{\text{left}}, \\ u_{\text{left}} \frac{1/2}{1 - v_{\text{left}}} & \text{if } v_{\text{left}} \leq 1/2 \quad \text{and} \quad v_{\text{right}} \geq 1/2. \end{cases} \quad (63)$$

On the coexistence line ($0 < v_{\text{right}} = 1 - v_{\text{left}} < 1/2$) the stationary v -profile is linear as known from the ASEP.^(23,24) This induces also a linear profile for u according to (61).

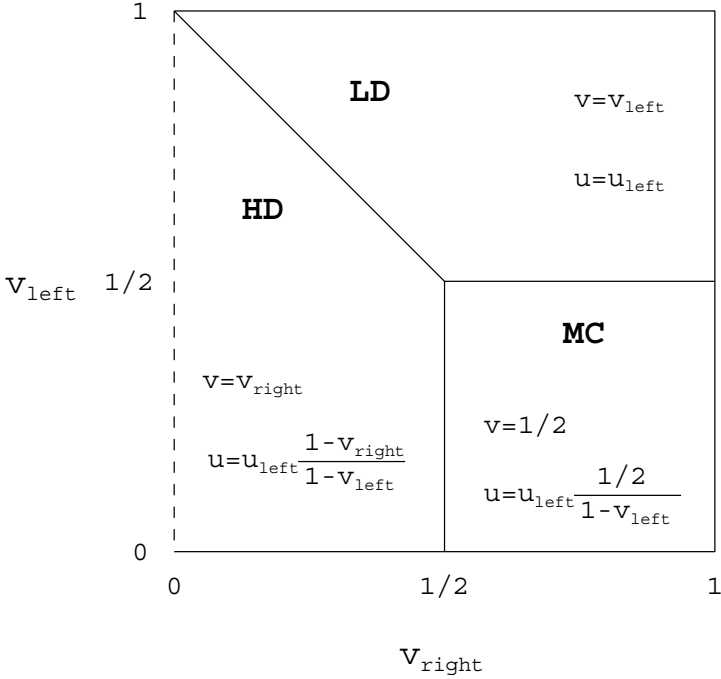


Fig. 5. The phase diagram of the open system. Since the vacancies follow the ASEP dynamics the boundary values of v determine the phase according to the ASEP phase diagram. In addition Eq (61) determines the stationary value of u in all phases except on the dashed line where one has symmetric diffusion of A and B resulting in linear profiles for u connecting $u_{\text{left}}/(1 - v_{\text{left}})$ and u_{right} .

If $v_{\text{right}} = 0$ then there are no vacancies in the system leading to symmetric diffusion of A and B particles. This results in linear profiles for u connecting $u_{\text{left}}/(1 - v_{\text{left}})$, which is the value of u after the discontinuity located at the left boundary, and u_{right} as expected from the symmetric exclusion process (SEP) ⁽²⁶⁾ and confirmed in Appendix A.

5. CONCLUSION

We have introduced an asymmetric exclusion process with two conserved species of particles. Its study is part of the program to understand the emergence of macroscopic behaviour from microscopic models of non-equilibrium diffusive interacting particles and to elucidate the significance of boundary conditions in driven diffusive systems. Under heuristic Eulerian scaling we obtain a system of PDEs which can be analysed analytically.

As one would have expected from the nonlinear current-density relation the system may produce shock discontinuities on the macroscopic scale. There are two types of shocks (as expected in systems with two conservation laws) for which we calculate the respective shock velocities and intermediate densities in terms of the asymptotic limiting densities.

The model we have introduced here allows for a rigorous analysis of the *microscopic* structure of a shock of type 1 (with a discontinuity in the vacancy density), provided that some special conditions on the hopping parameters and shock densities are satisfied. For this shock one finds the same behaviour as for the ASEP, suggesting that also for nongeneric values of the limiting densities of the shock the behaviour would be similar. Shocks of type 2 (constant vacancy density) are microscopically unstable, they correspond to diffusive spreading as in the symmetric exclusion process.

Part of our investigation is devoted to the problem of steady state selection in the open system.⁽²⁷⁾ Unlike for driven diffusive system with a single species of particles⁽¹⁶⁾ there is no developed theory of boundary-induced phase transitions for systems with two or more conservation laws. Using the known phase diagram of the ASEP and the microscopic properties of the shock in our particular model we have derived the stationary phase diagram. So our model, even though degenerate, may serve as a testing ground for any general theory. With a view on some of our earlier results on driven diffusive two-species systems with open boundaries we note that we found that the heuristic approach to steady-state selection of ref. 9 reproduces the independently derived phase diagram.

An intriguing observation is that the u -density in the phase diagram depends continuously on the left v -density throughout the maximal current phase. In order to explain the significance of this observation we note that the phase diagram of single-species systems can be predicted from the current-density relation in terms of *boundary densities*,^(21,22) which in general are unknown functions of the *boundary rates* of the model. On the other hand any numerical study of a given model yields the phase diagram in terms of the boundary rates, not the boundary densities. Therefore, a comparison between theoretical predictions and numerical observations requires knowledge of the nonuniversal relationship between boundary densities and boundary rates. In the ASEP and generally in single-species systems the order parameter (the bulk density) in the maximal current phase does not depend on the left boundary density. Hence it is not possible to measure the relationship between the left boundary density and the boundary rates of the model. This in turn makes it impossible to predict the phase diagram in terms of the boundary rates. In the present two-species model, however, the left boundary density can be measured in the

maximal current phase as a function of the system parameters through measuring u .

This leads to an unexpected offspin of our investigation: by regarding the two-species model as an exclusion process with two kinds of vacancies (by identifying vacancies with particles and the two kinds of particles with vacancies). Generalizing other single-species systems in a manner similar to what is done here, viz., leaving their dynamics unchanged by just introducing tagged diffusive vacancies, may provide a means of measuring those postulated boundary densities in terms of the model parameters even in parts of the phase diagram where the order parameter itself does not depend on the boundary densities.

Finally we remark that in principle the processes $A \rightarrow B$ or $B \rightarrow A$ could also be excluded (i.e. $\gamma_{l(r)}^{+(-)} = 0$) from our process. We only keep them for the sake of generality. If one wants to choose the boundary conditions to mimic certain boundary densities these rates are in general non-zero. However, in our model these processes don't play an important role unlike in the so-called bridge model where they are responsible for spontaneous symmetry breaking.⁽²⁸⁾ The precise mechanism for this phenomenon and a quantitative description, however, still remain a major challenge in the study of two-species systems with open boundaries.

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APPENDIX A. SOLUTION OF THE HYDRODYNAMIC EQUATIONS WITH FINITE VISCOSITY

The viscous hydrodynamic equations for the steady state coming from the method described in ref. 9 (see Section 4.3) are the following

$$(p - q)v'(2v - 1) = a \frac{p + q}{2} v'', \quad (64)$$

$$(p - q)(u'v + v'u) = a \frac{p + q}{2} (u''v - v''u) + ac((1 - v)u'' + uv''). \quad (65)$$

Substituting $u = (1 - v)\phi$ in (65) and using (64) we arrive at the following equation for ϕ

$$v(1-v)\phi' = \frac{a(p+q)}{2(p-q)} (v(1-v)\phi'' - 2vv'\phi') + \frac{ac}{p-q} \left((1-v)^2\phi'' - 2(1-v)\phi'v' \right). \quad (66)$$

One can immediately see here that $\phi = \text{const.}$ is a solution if it fits both boundaries, i.e., if $\phi_{\text{left}} = \phi_{\text{right}}$. When this does not hold (this is the case in general) then one has

$$\frac{d}{dx} \ln |\phi'| = \frac{2v'}{1-v} + \frac{v}{\frac{a}{p-q} \left(\frac{p+q}{2} v + c(1-v) \right)}. \quad (67)$$

Integrating from the right boundary we get

$$\begin{aligned} \ln |\phi'(y)| &= \ln |\phi'(1)| \\ &\quad - \int_y^1 \frac{v}{\frac{a}{p-q} \left(\frac{p+q}{2} v + c(1-v) \right)} dx \\ &\quad - 2 \int_{v(y)}^{v_{\text{right}}} \frac{dv}{1-v}. \end{aligned} \quad (68)$$

Assuming that the sign of ϕ' does not change in the system we arrive at

$$\begin{aligned} \phi'(y) &= \phi'(1) \left(\frac{1-v_{\text{right}}}{1-v(y)} \right)^2 \\ &\quad \times \exp \left(-\frac{p-q}{a} \int_y^1 \frac{v}{\frac{p+q}{2} v + c(1-v)} dx \right). \end{aligned} \quad (69)$$

For strictly positive v in the bulk of the system one has $\phi'(y) \rightarrow 0$ as $a \rightarrow 0$ for any fixed $y < 1$ thus the limiting ϕ profile is flat everywhere apart from the right boundary, which implies $\phi_{\text{bulk}} = \phi_{\text{left}}$.

There is no positive lower bound for v if and only if $v_{\text{right}} = 0$ (dashed line in Fig. 5). In this case $v(x) \rightarrow 0$ everywhere as $a \rightarrow 0$ apart from the left boundary (provided $v_{\text{left}} \neq 1$) which implies $\phi''(x) \rightarrow 0$ for any fixed $x > 0$ according to (66). We still have to show that ϕ does not have a discontinuity in the $a \rightarrow 0$ limit at the left boundary. For this we evaluate $\phi'(0)$ and show that it does not diverge. Similarly to (69) one has

$$\phi'(0) = \phi'_{\text{bulk}} \left(\frac{1}{1 - v_{\text{left}}} \right)^2 \times \exp \left(-\frac{p-q}{a} \int_0^y \frac{v}{\frac{p+q}{2}v + c(1-v)} dx \right), \quad (70)$$

where the upper limit of the integration $0 < y \leq 1$ is arbitrary because of the fast decay of the integrand. Since the integrand is non-negative the exponential cannot diverge which gives

$$\lim_{a \rightarrow 0} \phi'(0) < \infty. \quad (71)$$

This means that the ϕ profile is the linear function connecting the two boundary values. The u profile, however, has a discontinuity at the left boundary according to (53) and jumps from u_{left} to $u_{\text{left}}/(1 - v_{\text{left}})$. From here it goes linearly to the right boundary value u_{right} .

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