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**Markov Processes** and **Related Fields**


# Broken Ergodicity in Driven One-Dimensional Particle Systems with Short-Range Interaction

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**Abstract.** We present a one-dimensional nonequilibrium model for a driven diffusive system which has local interactions and slow nonconservative reaction kinetics. Monte-Carlo simulations suggest that in the thermodynamic limit the steady state exhibits a phase with broken ergodicity. We propose a hydrodynamic equation for the coarse-grained density (under Eulerian scaling), augmented by a prescription how to treat shock and boundary discontinuities, respectively. This conjecture can be readily generalized to other weakly nonconservative driven diffusive systems and is supported by a heuristic identification of the main dynamical mode that governs the microscopic dynamics, viz. the random motion of a shock in an self-organized effective potential. This picture leads to the exact phase diagram of the system and suggests a novel and mathematically tractable mechanism for "freezing by heating".

Keywords: broken ergodicity, nonequilibrium phase transition, asymmetric simple exclusion process, biological transport processes

AMS Subject Classification: 82C26, 82C70, 82C22, 60K35

## 1. Introduction

Over the last decade stochastic interacting particle systems have become a widely accepted tool for addressing not only applied but also fundamental problems of nonequilibrium statistical mechanics [1–3]. The closely related questions of phase coexistence and ergodicity breaking in noisy one-dimensional particle systems with short range interactions and finite local state space are particularly intriguing from a statistical mechanics perspective. In thermal equilibrium

these phenomena cannot occur as there is no local mechanism that could limit the growth of islands of a minority phase inside a majority phase. Far from equilibrium one has found phase separation and spontaneous symmetry breaking in driven diffusive systems provided that either a bulk conservation law, viz. particle number conservation [4–7,11,12], or vanishing local transition rates [8,9] constrain the local dynamics, for a review see [10].

On the other hand, it is known that mean-field approximations and numerical evidence for phase transitions in one-dimensional nonequilibrium systems [11,12] may be subtle and — as has been demonstrated by exact results — indeed be misleading [13–15]. This calls for rigorous mathematical treatment of the problem. A second issue that drives the interest in this problem comes from trying to understand whether in the absence of local constraints on the transition rates broken ergodicity may arise not only for rather complicated local dynamics [16–18] (involving a large local state space or interactions extending over finite, but rather large domains), but also in a more transparent manner in models which have a simple and natural microscopic motivation. Recently it has been shown that phase coexistence occurs in a one-dimensional driven diffusive system in the presence of Langmuir kinetics $A \rightleftharpoons 0$ which break the bulk conservation law [19]. This mechanism is inspired by the motion of motor proteins along actin filaments. Earlier this model was introduced as a toy model reproducing stylized facts in limit order markets [20]. The formation of a localized shock in this system which separates a domain of low particle density from a domain of high density has been studied subsequently [21, 22]. However, the two different domains are stabilized by judiciously chosen boundary conditions and thus do not represent two possible *global* steady states for the same set of boundary parameters. The process remains ergodic even in the thermodynamic limit.

Here we review recent results [23] that demonstrate the existence of broken ergodicity (in the thermodynamic limit) in a driven diffusive system without bulk conservation law and comment on some issues pertaining to the hydrodynamic limit for weakly nonconservative systems with open boundaries. Studying the system under Eulerian scaling we derive nonrigorously an exact nonconservative hydrodynamic equation which, together with a microscopically motivated prescription how to treat shock discontinuities and boundary layers, describes broken ergodicity on macroscopic scale.

## 2. The model and its steady state

To be specific we consider the totally asymmetric exclusion process (TASEP) augmented by nonconservative reaction kinetics. The TASEP is a stochastic model of diffusing particles on a one-dimensional lattice with a hopping bias in one direction [2, 3]. Each site from 1 to $L$ is either empty ('$\varnothing$') or occupied by one particle ('$A$'). The occupation number at lattice site $k$ is represented as a

stochastic variable $n_k = 0, 1$. In the bulk particles hop stochastically from site $i$ to $i+1$ with unit rate, provided that the target site is empty. The boundaries act as particle reservoirs with densities $\rho_-$ on the left resp. $\rho_+$ on the right: On site 1 particles are created with rate $\rho_-$, provided the site is empty, which corresponds to a particle hopping from the left reservoir onto the first site. Particles on site $L$ are annihilated with rate $1-\rho_+$, corresponding to a particle hopping from the last site into the right reservoir. The expected current $j_k$ across the bond $k, k+1$ for these hopping dynamics is given by the expectation value

$$j_k = \langle\, n_k(1-n_{k+1})\,\rangle. \tag{2.1}$$

The expected local density is denoted by $\rho_k = \langle\, n_k\,\rangle$.

In our model particles also undergo the following reaction process: On a vacant site enclosed by two particles a particle may be attached with rate $\omega_a$, and a particle enclosed by two other particles may be detached with rate $\omega_d$. This process can be symbolically written as

$$A\varnothing A \rightleftharpoons AAA$$

and may be interpreted as activated Langmuir kinetics. With periodic boundary conditions the process is trivially nonergodic. In particular, there are two invariant measures for this process which are product measures with density $\rho = \omega_a/(\omega_a+\omega_d)$ or zero respectively [24]. With open boundary conditions as defined above the process is ergodic and has a complicated invariant measure, to be studied below. The question we address is whether in the thermodynamic limit $L \to \infty$ nonergodicity can arise.

We consider the physically interesting case where the bulk reaction rates are proportional to $1/L$ [19–23]. Under this scaling the violation of particle conservation in the bulk is equal in strength with the violation at the boundaries and a competition between the two mechanisms sets in. We define renormalized rates

$$\omega_a = \Omega_a/L, \qquad \omega_d = \Omega_d/L \tag{2.2}$$

where $\Omega_a$ and $\Omega_d$ are kept constant while $L \to \infty$. With these dynamics the expected bulk density satisfies the equation

$$\frac{d}{dt}\rho_k + j_k - j_{k-1} = S_k \tag{2.3}$$

which is a lattice continuity equation with a source term

$$S_k = \frac{1}{L}\left[\Omega_a\langle\, n_{k-1}(1-n_k)n_{k+1}\,\rangle - \Omega_d\langle\, n_{k-1}n_kn_{k+1}\,\rangle\right]. \tag{2.4}$$

We find a stationary phase diagram of the model with five distinct phases (Figure 1). The stationary density profile $\rho_i$ is not constant as a function of

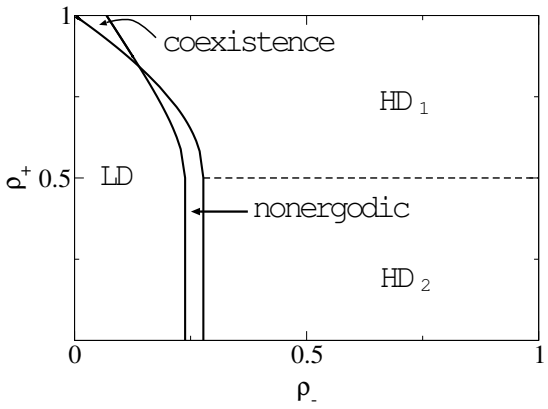


Figure 1. Phase diagram for $\Omega_a = 0.7$ and $\Omega_d = 0.1$ with two high density phases (HD1, HD2), a low density phase (LD), a coexistence phase and the nonergodic phase (from [23]).

lattice site $i$. Yet some of the phases are reminiscent of the usual TASEP with open boundaries [26–28]: in the high density phases (HD1/2) one finds $\rho_i > 1/2$ while in the low density phase (LD) $\rho_i < 1/2$. In HD1 the bulk density profile is dependent on $\rho_+$, while it is independent of both boundaries in HD2 as in the maximal current phase of the TASEP. On the other hand two additional phases exist: A coexistence phase which is characterized by a stable shock position, i.e., a jump in the density profile which is localized at a certain position in the bulk of the system. The shock connects a low density domain to its left with a high density domain to its right as known from related models studied previously [19, 21]. Notice that in the usual TASEP there is a coexistence line in the phase diagram with a *nonlocalized* shock [27, 31]. In a different parameter regime we find a novel phase with an unstable shock position in the bulk. In this phase both the LD and HD states are stable (if $L \to \infty$) for the same values of boundary densities which implies that ergodicity is broken in the thermodynamic limit. Although for finite systems a transition between the two states is possible, the mean life time of each steady state is exponentially large in the system size $L$ (see below). This phase has no analog in the TASEP with open boundaries. It is reminiscent of broken ergodicity in an Ising model below the critical temperature, but we note that there is no spontaneous symmetry breaking involved since there is no symmetry relating the two metastable states.

## 3. Hydrodynamic limit

In order to derive these observations we first consider the hydrodynamic limit on the Euler scale, i.e., we take $L \to \infty$ while the lattice constant is scaled by $a = 1/L$ and the time by $t = t_{\text{lattice}}/L$. Thus the spatial coordinate $x$ becomes continuous. We recall that in the exclusion process without reaction kinetics the system is locally stationary under this scaling in any finite region around some lattice point $k = x/a$. From a physical point of view this represents the key ingredient in the rigorous proof of the hydrodynamic limit of purely conservative particle systems [29] defined on an infinite lattice (for the rigorous hydrodynamics of the finite open system see [30]). Since the nonconservative part of the bulk dynamics of the system at microscopic scale is so slow that locally the system reaches stationarity with respect to the conservative part of the dynamics we argue that local stationarity also applies in the presence of slow dynamics as defined above. Any local perturbation caused by the nonconservative dynamics would dissipate before interacting with another local perturbation, thus leaving correlations in the locally stationary state unperturbed on long time scales. Only mass flow occurs, allowing for a macroscopically varying density. (For physical insight in the formation of shocks one needs some other tools which are discussed below.)

Hence, using (2.3), for our model the hydrodynamic equation for the coarse grained density takes the form

$$\frac{\partial}{\partial t}\rho(x,t) + \frac{\partial}{\partial x}j(\rho) = S(\rho), \tag{3.1}$$

with the exact current $j(\rho) = \rho(1-\rho)$ of the TASEP and the cubic source term

$$S(\rho) = \Omega_a \rho^2(1-\rho) - \Omega_d \rho^3 \tag{3.2}$$

resulting from the activated Langmuir kinetics. This term is calculated from (2.4) and the invariant product measure of the pure ASEP which also enters in the calculation of the current. We remark that for more general hopping dynamics augmented by slow reaction kinetics the structure of the hydrodynamic equation remains identical, but the current and the source term are functions of the particle density $\rho$ which have to be evaluated as expectations of the corresponding microscopic quantities with respect to the invariant measure of the pure hopping dynamics.

For the stationary state $\partial_t \rho(x,t) = 0$ holds and using $\partial_x j = \partial j/\partial\rho \cdot \partial\rho/\partial x$ we obtain

$$v_c(\rho)\,\frac{\partial \rho(x)}{\partial x} = S(\rho), \tag{3.3}$$

with the collective velocity $v_c = \partial j/\partial\rho$. This nonlinear differential equation can be integrated analytically and yields the flow field

$$x(\rho) = -\frac{1}{\Omega_a \rho} + \frac{\Omega_a - \Omega_d}{\Omega_a^2} \ln\left|\frac{1}{K} - \frac{1}{\rho}\right| + c \tag{3.4}$$

with an integration constant $c$.

As the differential equation is of first order and the boundary condition fixes the density at two positions, following a line of the flow field does not represent a solution of the boundary problem in general. In the original lattice model this inconsistency is resolved by the appearance of a shock and/or boundary layers as described below. Apart from the discontinuities the stationary density profile follows the flow field of equation (3.3).

The discontinuities are determined by the following set of rules [21]:

(A) In the interior of the lattice the stationary density profile either follows a line of the flow field of the differential equation (3.3) or makes a jump. Jumps can only occur between densities yielding the same current, i.e., *the current $j(\rho(x))$ 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:

$$\rho'_- = \lim_{x\to+0} \rho(x), \quad \rho'_+ = \lim_{x\to1-0} \rho(x),$$

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:

$$\text{if } \rho_- < \rho'_-, \text{ then } j(\rho) > j(\rho'_-) \text{ for any } \rho \in (\rho_-, \rho'_-), \tag{3.5}$$
$$\text{if } \rho_- > \rho'_-, \text{ then } j(\rho) < j(\rho'_-) \text{ for any } \rho \in (\rho'_-, \rho_-). \tag{3.6}$$

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

$$\text{if } \rho'_+ < \rho_+, \text{ then } j(\rho'_+) < j(\rho) \text{ for any } \rho \in (\rho'_+, \rho_+), \tag{3.7}$$
$$\text{if } \rho'_+ > \rho_+, \text{ then } j(\rho'_+) > j(\rho) \text{ for any } \rho \in (\rho_+, \rho'_+). \tag{3.8}$$

(C) Shocks between a density $\rho_l$ to the left of the shock and $\rho_r$ to the right of the shock are stable only if they are stable in the absence of reaction kinetics [34].

For the special case of the TASEP with simple Langmuir reaction kinetics similar rules have been postulated in [19].

## 4. Microscopic heuristics

Outside the regime of broken ergodicity the rules (A)–(C) define a unique solution which correctly describes the numerically observed phase diagram. As a way to derive these rules one may take a phenomenological approach and add an infinitesimal viscosity term that regularizes the nonlinear hydrodynamic equation. However, these rules can also be derived from microscopic considerations which we expect to be valid quite generally. Following [21] we first consider the effect of an infinitesimal viscosity and observe the following.

- Although the reaction kinetics does not conserve locally the number of particles, equation (3.1) with an infinitesimal viscosity added can be rewritten formally in the form

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial}{\partial x}\,\tilde{j}(x,t) = 0 \tag{4.1}$$

with

$$\tilde{j}(x,t) = j(\rho) - \int_A^x \mathcal{L}(\rho)\,dx - \nu\,\frac{\partial \rho}{\partial x} - \mathcal{F}(t) \tag{4.2}$$

where $\mathcal{F}(t)$ is some time-dependent integration constant. Suppose that there is a shock at the position $X_0$ connecting the densities $\rho_l$ and $\rho_r$. The mass transfer across the shock is

$$\begin{aligned} \frac{\partial}{\partial t}\int_{X_0-0}^{X_0+0} \rho(x,t)dx &= \tilde{j}(X_0+0,t) - \tilde{j}(X_0-0,t) \\ &= j(\rho_r) - j(\rho_l), \end{aligned} \tag{4.3}$$

since the Langmuir term and the viscosity term change only infinitesimally across the shock. In the stationary state, the RHS of (4.3) vanishes which explains the rule (A).

- Rule (B) is due to the fact that in the boundary layer of vanishing length the reaction term can be neglected. Thus for the stationary current at the boundaries we have $\tilde{j}(x) = j(\rho(x)) - \nu(\partial\rho/\partial x) = J$, which is equivalent to rule (B). Indeed at the left boundary $J = j(\rho'_-)$ (see (3.5) 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 (3.5). Analogously one obtains (3.6)–(3.8).

- The rule (C) is explained by the marginal role the reaction kinetics plays locally in space and in time and by observing that it is not affecting directly the particle motion. Hence, the local perturbations will still spread with the velocity corresponding to the local density level $\rho$, thus rendering the

same stability conditions for a shock as for the diffusive system without reaction kinetics [3].

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 [33, 34]. 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 reaction kinetics.

One realizes that for certain values of boundary densities the rules (A)–(C) give several possible solutions with different types of discontinuities. In particular, there is a range of boundary densities which allow for three different solutions with the shock either in the bulk or at one of the two boundaries. This suggests that the occurrence of broken ergodicity is linked with the presence of a shock discontinuity. In order to understand quantitatively the selection of the stationary shock position from a microscopic viewpoint we need to consider the effect of fluctuations. We propose to describe the dominant dynamical mode of the particle system that drives the system into the stationary state in terms of the random motion of the shock. To this end we view the shock as a point object and generalize the approach of [31] and introduce space-dependent hopping rates

$$w_{x\to x+a} = \frac{j_R(x)}{\rho_R(x) - \rho_L(x)},$$
$$w_{x+a\to x} = \frac{j_L(x)}{\rho_R(x) - \rho_L(x)} \tag{4.4}$$

for jumps of the shock over a lattice constant $a$. Here the indices $L$ and $R$ denote the solutions (lines of the flow field (3.4)) on the left, resp. right, of the shock. Similar hopping rates are used in [22]. The space-dependent hopping rates furnish us with the picture of a random walker in an effective energy landscape $E(x)$ inside a finite box. The energy landscape is generated by the interplay of the particle current with the reaction kinetics. In this way we relate the original nonequilibrium many-particle system to an equilibrium single-particle model. Let $p(x)$ be the equilibrium probability of the shock being at position $x$. Then due to detailed balance

$$\frac{w_{x\to x+a}}{w_{x+a\to x}} = \frac{p(x+a)}{p(x)} = \exp(-E(x+a) + E(x)). \tag{4.5}$$

which defines the energy landscape.

The potential $E(x)$ is a monotonically increasing (decreasing) function for the HD (LD) phase (Figure 2). This implies that although there are fluctuations the shock is always driven to the left (right) boundary. In the coexistence phase there is a global minimum in the bulk resulting in a stable shock position

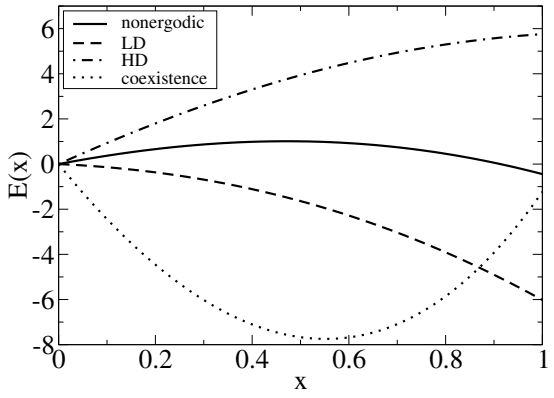


Figure 2. Examples for the energy landscape in four phases. Note that in the HD and LD phases $E(x)$ can be either convex or concave. (From [23].)

(Figure 2) at a macroscopic distance from the boundaries. Here the dynamics can be well approximated by a random walker in a harmonic potential which gives a Gaussian distribution for the shock position. Hence the width of the shock distribution is proportional to $\sqrt{L}$ [24] which was also found in [19, 22] for the TASEP with Langmuir kinetics.

The nonergodic phase is characterized by a global energy *maximum* in the bulk (Figure 2), leading to an unstable bulk fixed point of the shock. The two minima at the left and right boundary correspond to the two stable stationary states. Starting with an initial condition close to one of the minima, the random walker will drift most likely into this local minimum and stay in its vicinity for a time of the order of the mean first passage time $\bar{\tau}$ before it traverses to the other minimum. Using a formula for the mean first passage time derived by Murthy and Kehr [35] one expects that $\bar{\tau}$ grows exponentially with the system size $L$. Moreover, one expects the transition from one minimum to the other to be a random Poisson process with an average waiting time $\bar{\tau}$ [24].

This simple one-particle picture is well borne out by MC simulations. For judiciously chosen parameters it is possible to perform simulations up to times much larger than $\bar{\tau}$. Using multispin coding [36] for the MC algorithm rather good statistics become available for the waiting time $\tau$ (the time the system spends in one of the stationary states before switching to the other). For tracing the position of the shock on the lattice scale with the second–class particle technique [37], which we adapt to allow for reactions to take place [24]. We measured the position of the second–class particle as a function of time: a typical

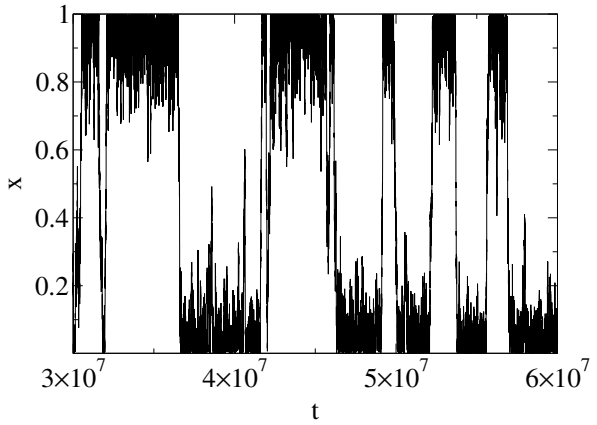


Figure 3. Snapshot of the time evolution of the scaled position of the second–class particle for $L = 1000, \rho_- = 0.2705, \rho_+ = 0.63, \Omega_a = 0.5, \Omega_d = 0.1$. A position of the second-class particle near the left boundary ($x \approx 0$) corresponds to the high density state, while a position near the right boundary ($x \approx 1$) corresponds to the low density state. (From [23].)

realization is shown in Figure 3. The numerically determined cumulative distribution function $\Phi(t) = P(\tau < t)$ of the waiting time $\tau$ is hardly distinguishable from an exponential distribution [23].

With this picture of a moving shock in mind and using the expression (3.4) it is possible to derive the exact phase transition lines defining the phase diagram presented above. The sign of the slope of the energy profile, i.e., the stability of the shock position can be analyzed by considering the average shock velocity

$$v_s(x) = \frac{j_R(x) - j_L(x)}{\rho_R(x) - \rho_L(x)}. \tag{4.6}$$

A shock position at the boundary is stable when it is driven towards the boundary, i.e., $v_s(0) < 0$ at the left, $v_s(1) > 0$ at the right boundary. Thus the lines separating the phases are calculated by comparing the values of $\rho_L(x)$ and $\rho_R(x)$ at the positions $x = 0, 1$. In the high- and low-density phase respectively the energy profile has a unique minimum at one of the boundaries. In the nonergodic phase the energy profile exhibits two minima at the boundaries, so that the shock position is stable at both of them.

We mention in passing that the analytical treatment predicts a phase near the intersection point of the two nontrivial lines in the phase diagram with an energy profile having a minimum and also a maximum in the bulk. However

the region in the $(\rho_-, \rho_+)$ space is rather narrow and the energy landscape is too flat to observe this in simulations. For a more detailed discussion, see [24].

## 5. Conclusions

We have presented a simple nonequilibrium system with local non-conservative dynamics and finite local state space which exhibits ergodicity breaking in the thermodynamic limit, in the usual sense that in finite volume the sojourn time in two metastable steady states increases exponentially with system size. The description of the nonequilibrium many-body dynamics in terms of a collective single-particle mode moving under equilibrium conditions yields the exact stationary phase diagram as well as the numerically verified flipping process between the metastable states of the finite system. The two different stationary distributions are not ordered states in which the activated Langmuir reaction kinetics would be dynamically suppressed.

In order to avoid misinterpretation of our approach and its central result, viz. the hydrodynamic equation (3.1) along with rules (A)–(C), we stress that in our derivation we do not employ a mean field approximation, as appears to be believed in [25]. We neither neglect any noise implicit in the underlying stochastic dynamics, (the effects of which disappear under Eulerian scaling but can be observed on finer scales e.g. as shock fluctuations, see above), nor do we propose to make any approximation in the evaluation of the current and source term respectively as functions of the density $\rho$. In fact, our approach assumes that the *exact* invariant measure of the pure hopping process is known at least to the extent that the macroscopic current and the source term can be calculated exactly as function of the density. Any mean-field approximation for these quantities would lead to wrong results, unless the exact stationary measure is simple (e.g. product measure) and mean-field theory happens to produce the correct result. Generically, however, this is not the case. That such an approximation could actually be entirely misleading can readily be demonstrated for KLS-hopping dynamics, where the exact invariant measure is an Ising measure [32, 33]. KLS dynamics are the most natural generalization of the ASEP, involving next-nearest neighbor interactions. For sufficiently strong interaction strength the current looses convexity (as a function of $\rho$) and develops two local maxima. The result is far more complex phase diagram with more phases than in the ASEP, both with [21] or without reaction kinetics [33, 34]. However, a simple mean field approximation neglecting all correlations (which works for the TASEP because the exact invariant measure is product and thus has no correlations) would predict that phase diagram for the ASEP and the KLS model are the same!

From a physical viewpoint our main result is intriguing for two distinct reasons. Firstly, it is somewhat counterintuitive that adding weak noise which breaks the conservation law results in broken ergodicity which is absent in

the conservative system. This is reminiscent of, but distinct from mean-field type stochastic dynamics with infinitely fast hopping rates. For infinitely fast hopping the density profile of an open system would be macroscopically flat, whereas under our scaling the density profile is a nontrivial function of continuous space. Moreover, one expects for infinitely fast hopping that the phase diagram would be boundary-determined, reducing to that of the pure hopping process with open boundaries, where no broken ergodicity occurs. Secondly, we find it interesting that a noisy dynamics which is on average spatially homogeneous (the nonconservative reaction process) added to a conservative spatially homogeneous nonequilibrium system with boundaries leads to a *space-dependent* effective force which determines the stationary position of the shock. In the absence of this noise, i.e., in the usual TASEP, the shock performs an unbiased random walk at the first-order phase transition line and hence is unlocalized, whereas suitably chosen reaction kinetics may create a variety of effective potentials which localize the shock in the bulk. An increase in noise strength is usually associated with heating up a system whereas localization reduces the amount of disorder, corresponding to cooling. Thus we are faced with novel mechanism for "cooling by heating". The rigorous derivation of the hydrodynamic limit remains an open problem.

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