

Fixed points and boundary layers in asymmetric simple exclusion processes

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In this paper, we show how a fixed-point-based boundary layer analysis can be used to understand phases and phase transitions in asymmetric simple exclusion processes (ASEPs) with open boundaries. In order to illustrate this method, we choose a two-species ASEP which has interesting phase transitions not seen in the one-species case. We also apply this method to the single-species problem where the analysis is simple but nevertheless quite insightful.

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Asymmetric simple exclusion process (ASEP) [1] in its simplest form involves particles moving on a one-dimensional (1D) lattice with a bias in one specific direction. Due to the mutual exclusion rule, the occupancy of a site by more than one particle is ruled out. The biased motion of particles is responsible for a particle current which is a typical indication of the system being away from the thermodynamic equilibrium. With open boundaries, the system needs to be coupled to particle reservoirs, which maintain constant densities at the boundaries. All these nonequilibrium systems after sufficiently long time settle in a steady state where properties such as the average density of particles, current, etc. are independent of time. A striking feature of the open system is the boundary-induced phase transition where the tuning parameters are the boundary densities [2]. Various bulk phases characterized through distinct current or particle-density profiles are usually represented in a phase diagram in the space of the boundary densities.

Unlike equilibrium systems which carry no current, for ASEP, the information about the change in the boundary condition (BC) is mediated up to the bulk by the particle current. Therefore, the issue as how the BCs affect the boundary layers holds the key to understand the boundary-induced phase transitions in ASEP. Recent studies [3–5] have shown that the boundary layer analysis is a very general approach to probe different models of ASEP. In this approach, starting with the steady-state hydrodynamic equation, a uniform approximation for the density valid both in the bulk and in the boundary region is developed. For particle nonconserving ASEP, this method shows that the formation of a discontinuity in the bulk-density profile (or a localized shock) is due to a deconfinement of a boundary layer from the boundary. This deconfinement is shown to be associated with the divergence of the width of the boundary layer [3].

In this paper, we show how a fixed-point description of the boundary layers and the phase-plane trajectories connecting the fixed points can be used to map the bulk phase diagram and identify the phase transitions. As an example, this method is applied to a particle-number-conserving ASEP that involves two species of particles [6]. In addition, we also consider the single-species system, where the analysis is especially simple.

In the two-species model considered in this paper, particles, denoted by A and B , move in opposite directions on a 1D lattice of length L with N lattice points obeying the fol-

lowing hopping rules: $A0 \rightarrow 0A$ with rate 1, $0B \rightarrow B0$ with rate 1, and $AB \rightarrow BA$ with rate 2. Here 0 denotes an empty lattice site. While A -type particles are injected (withdrawn) at the left (right) boundary, the reverse happens for B -type particles at these boundaries. We assume that these injection and withdrawal rates effectively correspond to boundary reservoirs with fixed particle densities, which are the BCs for our problem. Two-species models with specific boundary rates are known for spontaneous symmetry breaking between the two species even when their dynamics is completely symmetric [7]. While systems specified through boundary rates show spontaneous symmetry breaking, this is not seen in systems specified through boundary reservoir densities [8]. Our analysis is valid for arbitrary boundary densities. Domain-wall-based studies with boundary densities [8] predict two first-order transitions taking the system from a low- to a high-density jammed phase via an intermediate phase which is not seen in single-species systems. (See also Ref. [9].) In the steady state, the particle number conservation leads to a flat density profile in the bulk. Domain-wall arguments show that unlike the high- or low-density phase where, as in the single-species case, the bulk densities are same as one of the boundary densities, the intermediate phase has bulk density not directly related to the boundary densities. Thus, it is important to understand what basic mechanism can be responsible for the existence of an intermediate phase and how the value of the bulk density in this phase is selected. The fixed-point description presented here unveils these issues.

The hydrodynamic formulation begins with the statistical averaging of the master equation that describes the time evolution of the probabilities of a given site occupied by either one of the two types of particles. A continuum limit, as the lattice spacing, $a \rightarrow 0$ and $N \rightarrow \infty$ with $L = Na$ remaining finite, is then taken for the resulting equation. The differential equations, thus obtained, involve the average particle densities $\rho(x, t)$ and $\eta(x, t)$ for A - and B -type particles with x and t as continuous variables representing position and time and the corresponding current densities j_ρ and j_η as functions of ρ and η . In the first order in $\epsilon = a/2$, the continuum equations are

$$\frac{\partial \rho}{\partial t} + \frac{\partial j_\rho}{\partial x} = \epsilon \frac{\partial}{\partial x} \left((1 + \eta) \frac{\partial \rho}{\partial x} - \rho \frac{\partial \eta}{\partial x} \right), \quad (1)$$

$$\frac{\partial \eta}{\partial t} + \frac{\partial j_\eta}{\partial x} = \epsilon \frac{\partial}{\partial x} \left((-\eta) \frac{\partial \rho}{\partial x} + (1 + \rho) \frac{\partial \eta}{\partial x} \right). \quad (2)$$

The stationary state of the model on a ring is given by a product measure and the exact stationary fluxes j_ρ and j_η are $j_\rho = \rho(1 - \rho + \eta)$ and $j_\eta = -\eta(1 - \eta + \rho)$.

The diffusionlike terms in Eqs. (1) and (2) are small in the $\epsilon \rightarrow 0$ limit. However, these terms are crucial for generating uniform approximations of the solutions. The stationary bulk densities (ρ_b and η_b) of constant values satisfy the differential equations trivially. These constant solutions cannot satisfy the BCs at both the ends. In order to satisfy the BCs, boundary layers are formed over narrow regions near one or both the boundaries [12]. To focus on this narrow region, we need to scale the position variable x as $\tilde{x} = (x - x_0)/\epsilon$, where x_0 specifies the location of the boundary layer, and express the stationary equations in terms of this new variable. Here, $x_0 = 0(1)$ for left (right) boundary layer which merges to the bulk particle-density profile asymptotically as $\tilde{x} \rightarrow +\infty$ ($-\infty$). A little algebraic manipulation and integrations of the stationary versions of Eqs. (1) and (2) lead to

$$p'(\tilde{x}) = c + q(1 - p),$$

$$(1 + p)q'(\tilde{x}) = d + p + q(c - pq), \quad (3)$$

where $p = \rho + \eta$ and $q = \rho - \eta$ with values lying within the ranges $[0, 1]$ and $[-1, 1]$, respectively. Here, prime denotes a derivative with respect to \tilde{x} and c and d are the integration constants. The saturation of the boundary layers located, for example, near $x = L$, to bulk as $\tilde{x} \rightarrow -\infty$, requires $c = -q_b(1 - p_b)$ and $d = q_b^2 - p_b$, where p_b and q_b are the bulk values of p and q , respectively. Since the bulk profile is flat, same c and d are applicable in case of boundary layers appearing near both the boundaries. For particle nonconserving systems, where the bulk profile is x dependent, p_b and q_b are the values of p and q at the point where the boundary layer merges the bulk. Although this approach is applicable to particle nonconserving systems, we restrict to the conserved case to avoid algebraic complications. Because of same c and d and the translational invariance, the same phase portrait is applicable to both the boundaries.

To understand the origin of the three phases, it is useful to study the stability properties of the fixed points of equations in Eq. (3). A combined single first-order differential equation involving $\frac{dp}{dq}$ leads to the solution $p(q)$ as a function of q , for a given BC at $x = 1$ or 0 . These solutions are the phase-plane trajectories flowing to the appropriate fixed points. The boundary layers are these trajectories seen as functions of \tilde{x} . Since these flows approach the fixed points in $\tilde{x} \rightarrow \pm\infty$, the bulk densities correspond to one fixed point. Also, by the choice of the constants c and d , the equations are guaranteed to have a fixed point that corresponds to the bulk densities. There exists three fixed points (p^*, q^*) , which are the solutions of the equations

$$p^* = (c + q^*)/q^*, \quad (q^*)^3 - (d + 1)q^* - c = 0. \quad (4)$$

Although the physically acceptable range of both c and d is $[-1, 1]$, there is only a narrow window in this c - d space (see the striped region in Fig. 1), where the fixed points can rep-

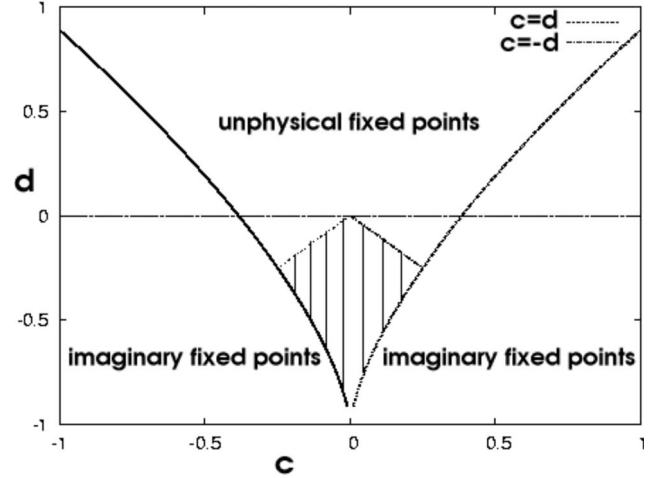


FIG. 1. Nature of the fixed points in the physically acceptable range of the c - d plane. On the bold solid line and the dashed line the discriminant of Eq. (4) is zero. Fixed points are imaginary in the region outside these two lines. In the striped region enclosed by these lines and the lines $d = c$ and $d = -c$, there are physically acceptable fixed points. In the rest of the space, not a single fixed point in the set of three has any physically acceptable value.

resent a meaningful density profile (within the physical domain, i.e., the values of p and q lie in the ranges $[0, 1]$ and $[-1, 1]$, respectively, and $0 \leq \rho, \eta \leq 1$).

Outside this window, the fixed points are either imaginary or do not have a single member that can represent the bulk. A stability analysis shows that out of the three fixed points, one is unstable, one is saddle, and one is stable. Based on their locations on the p - q plane, we call the stable and unstable fixed points as right (R) or left (L). The saddle fixed point is always denoted as S.

There exist the following possibilities:

(1) L is unstable and lies within the physical domain and R is stable with complex conjugate eigenvalues having negative real parts (spirally inward flow). R remains outside the physical domain and the bulk is, therefore, given by the L fixed-point values. The bulk in this case is also the same as the left BC. The right BC is satisfied by a boundary layer which is a part of the trajectory on the p - q plane starting from L and reaching the stable fixed point R. R is outside the physical range of p so that any physical BC is satisfied by the right boundary layer. Trajectories corresponding to different BCs at $x = 1$ are shown in Fig. 2(A).

(2) R is stable and lies within the physical domain and L is unstable with complex conjugate eigenvalues (spirally outward flow) having positive real parts. By the above argument, here the bulk satisfies the right BC with a boundary layer at $x = 0$ satisfying the left BC. The L fixed point must lie outside the physical domain. The trajectories in this case are shown in Fig. 2(B).

(3) There exists another situation where the saddle fixed point and either one of R or L is in the physical domain but the latter is different from the BC. In this case, the boundary layers should be described by the separatrices such that the bulk densities can acquire the saddle fixed-point values. BCs at both the boundaries are satisfied by boundary layers which

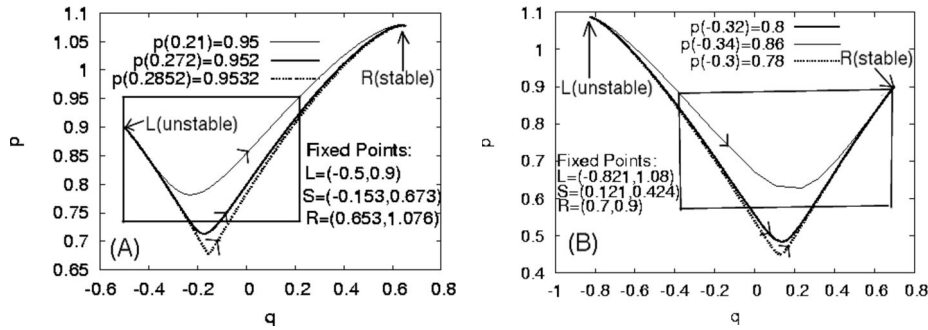


FIG. 2. Flow trajectories to the stable fixed point (R) with the BCs as specified in figure. Arrows indicate the direction of increasing x . (A) $c=0.05$ and $d=-0.65$ with BCs specified at $x=1$. (B) $c=-0.07$ and $d=-0.41$ with BCs at $x=0$. The rectangular boxes enclose portions of the trajectories with the BCs $\rho(0.21)=0.95$ for (A) and $\rho(-0.34)=0.86$ for (B). The length of the box is fixed by the fixed point in the physical domain and the BC of the specific trajectory it encloses. The vertical width of the box is chosen in such a way that it encloses the relevant part of the trajectory of interest. These parts of the trajectories in (A) [(B)] are seen as the right (left) boundary layers in ρ - x and η - x planes.

are parts of the separatrices joining L with S, and R with S. This phase where the bulk values of ρ and η are given by the saddle fixed-point values is the intermediate phase.

A general inspection regarding the stability of the fixed points in the allowed range of the c - d plane confirms these rules as the only possibilities. It also indicates that, for $c > 0$ ($c < 0$), the system remains either in L (R) or in the intermediate phase. In general, the intermediate phase appears when S is the only fixed point that lies in the domain specified by the BC.

The three rules mentioned above completely decide the phases and the phase boundaries. Suppose, we are in the left phase where the bulk densities are same as the left BCs. This allows us to calculate c and d , and thereby, the explicit values of all the three fixed points. The fixed point corresponding to the bulk-density values is an unstable one and the boundary layer solutions approach these values as $\tilde{x} \rightarrow -\infty$ while approaching the stable fixed point, which lies beyond the physical region, as $\tilde{x} \rightarrow \infty$. The boundary layers, which are part of the trajectories in Fig. 2, appear as in Fig. 3 in the ρ - x or η - x plane. The trajectories deviate because of the proximity of the saddle fixed point and this deviation appears

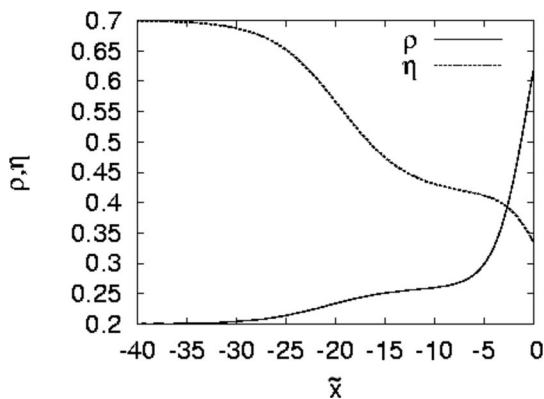


FIG. 3. Numerical solutions for the boundary layers in the L phase near $x=1$ for $c=0.05$ and $d=-0.65$. The boundary layers of ρ and η profiles merge to the bulk values of 0.2 and 0.7, respectively. The solutions tend to saturate to the saddle fixed point given by $(q, \rho) = (-0.153, 0.673)$.

as the tendency of the boundary layer to saturate to an intermediate value.

As the right BC is changed further keeping the left one unchanged, the solutions still appear like those of Fig. 2 or Fig. 3 with same bulk densities until a cusp appears in the trajectory. At this right BC, the trajectory is just the separatrix joining the unstable and the saddle fixed points on one side and the saddle and the stable fixed points on the other side. Since the flow now meets the saddle fixed point, the bulk densities are given by the saddle fixed-point values. This requires formation of a new boundary layer near $x=0$ with the height $\rho_u^* - \rho_s^*$, where ρ_u^* and ρ_s^* are the values of ρ at the unstable and the saddle fixed points, respectively. At this point, the system enters the intermediate phase. Since the values of the fixed points depend only on c and d or on the bulk density in the L phase, the height of the newly formed boundary layer is only dependent on the bulk density (or on c and d) of the L phase. The variation of the height of these new boundary layers with d for a given c is shown in Fig. 4.

The formation of a new boundary layer with a finite height and a discontinuous change in the value of the bulk density are indications of a first-order phase transition. This basic principle of the bulk densities acquiring the saddle fixed-point values continues to hold good inside the interme-

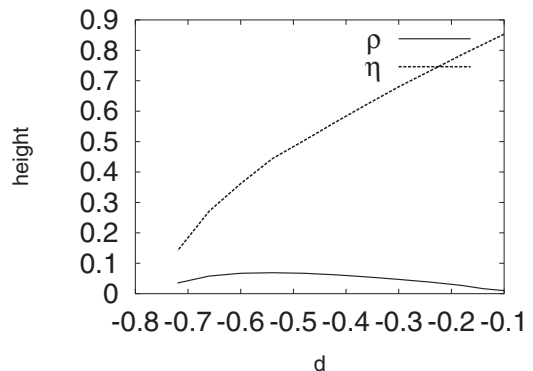


FIG. 4. Heights of the newly formed boundary layers at $x=0$ in the ρ and η profiles are plotted with d for $c=0.05$. These boundary layers are formed at the phase boundary between the L and the intermediate phases.

diate phase. In this phase, as the right BC is changed, the bulk values p_b and q_b change with boundary layers appearing at both the boundaries. The two boundary layers are the two separatrices joining the saddle fixed point to the stable and unstable fixed points. The bulk densities or the values of c and d are such that the right and left BCs lie exactly on these two separatrices.

Next, we apply this method to ASEP with only one kind of particles moving rightward on a 1D lattice obeying mutual exclusion. In the steady state, there are three phases depending on the left and right boundary densities α and $1-\beta$ [10], with the bulk particle density ρ_b being $\rho_b=1-\beta$, for $\alpha>\beta$ and $\beta<1/2$, $\rho_b=\alpha$, for $\beta>\alpha$ and $\alpha<1/2$, and $\rho_b=1/2$, for $\alpha>1/2$ and $\beta>1/2$. The approach to these phases can be understood well through the motion of the domain walls [11] which separate possible steady states of the system.

The equation that describes the boundary layer in this case is

$$(1/2)\rho'(\tilde{x}) = \rho(1-\rho) + c, \quad (5)$$

where the constant c is chosen as $c=-\rho_b(1-\rho_b)$ to assure saturation of the boundary layer to the bulk as $\tilde{x}\rightarrow\infty$ or $-\infty$. This equation has two fixed points $\rho^*=\rho_b, 1-\rho_b$. A stability analysis around these fixed points shows that (i) ρ_b is stable for $\rho_b>1/2$ and (ii) $1-\rho_b$ is stable if $\rho_b<1/2$.

In case of $\rho_b>1/2$, if a boundary layer has to saturate to ρ_b (the stable fixed point), its location should be at $x=0$. As $\tilde{x}\rightarrow-\infty$, this boundary layer saturates to the unstable fixed point $1-\rho_b$. The right BC is satisfied if $\rho_b=1-\beta$. Two conditions naturally follow from this: (i) $1-\beta>1/2$ or $\beta<1/2$ and (ii) $\alpha>1-\rho_b$ or $\alpha>\beta$, so that any boundary layer at $x=0$ satisfies the BC before saturating to the fixed point $1-\rho_b$. Similarly, in case of $\rho_b<1/2$, the boundary layer saturates to $1-\rho_b$ as $\tilde{x}\rightarrow\infty$ or ρ_b as $x\rightarrow-\infty$. A boundary layer of this nature should be located at $x=1$ with the conditions (i) $\alpha<1/2$ and (ii) $1-\rho_b>1-\beta$ or $\alpha<\beta$. As we see here, the location of the boundary layer is completely determined by the limit in which the bulk fixed point is approached by the

solution. In both $\rho_b>1/2$ and $\rho_b<1/2$ cases, while the boundary layers continue to be in the same position, their slopes change across the line $\alpha=1-\beta$. These boundary layers correspond to a different set of solutions of Eq. (5) and they approach the bulk fixed points at the same limits of \tilde{x} as before with opposite slopes. In general, the boundary layers saturating to two different densities are like localized domain walls of Ref. [11] separating two possible steady states. For $\rho_b=1/2$, the two fixed points merge and it is easy to see that the boundary layers from both sides of the system are able to approach the bulk density in a power-law fashion as $\sim\frac{1}{|\tilde{x}|}$ either as $\tilde{x}\rightarrow\infty$ or as $\tilde{x}\rightarrow-\infty$. Thus, in this case, there are boundary layers at both the boundaries. From a stability-analysislike approach, it is easy to see that both the boundary layers have negative slopes. This implies that such a phase is possible when $\alpha>1/2$ and $\beta>1/2$. These three possibilities cover the entire α - β parameter space.

In this paper, we show how a phase-plane analysis of the differential equations for the boundary layers can be used to predict boundary-induced phase transitions in ASEP. This method is applied to single-species as well as two-species processes. We arrive at a general prediction that for flat bulk profiles, the bulk densities in different phases are given by various fixed-point values of the differential equations describing the boundary layers. For two-species case, we find out the bulk density of the intermediate phase which has no one-species analog. The fixed-point analysis determines the nature of the transitions, the location of the boundary layers, and how the boundary layers merge to the bulk densities. For nonconstant bulk density, the fixed point of the boundary layer should match with the bulk-density value near their merging. In addition, we believe that this method can be applied to more complicated systems, such as those with more than two species of particles and the number of phase transitions can be predicted from the locations of the fixed points on the phase plane. The generality of the method suggests its wider applicability to various other systems where boundary-induced transitions can be seen.

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