Duality in one dimensional transport: Boundary layer approach

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ABSTRACT: We discuss the duality between the bulk phase transition and a boundary transition in nonequilibrium asymmetric exclusion process. By using a continuum description, it is shown that the bulk phase transitions can be understood as a deconfinement of a boundary layer, to be called the shockening transition. The duality gives the nature of the phase diagram and the exponents, especially near critical points for shock formation. This is also applied in an interacting model to study the nature of a nonequilibrium tricritical point.

Keywords: Nonequilibrium phase transitions, duality, tricriticality

1 INTRODUCTION

Our purpose in this paper is to show that boundary layers can be used to understand both qualitatively and quantitatively the bulk phase transitions in steady states of a class of nonequilibrium systems. The systems we have in mind are the well-studied asymmetric exclusion process (ASEP) with interacting particles.
The problem with nonequilibrium system is the absence of any Gibbs-Boltzmann type distribution, quite often because of absence of any hamiltonian. An associated problem is the definition of conjugate variables. because such pairs in equilibrium (analogs of pressure - volume type pairs) are defined via derivatives of the free energy. Nonetheless, the steady states are close cousins of the equilibrium states. The nature of the steady states can be changed by tuning the parameters of the system and this leads to the possibility of nonequilibrium phase transitions. The resulting phases can be represented in a phase diagram in the relevant parameter space. An important feature is that the bulk phase transitions are boundary driven - a phenomenon not found in equilibrium in general.
Bulk phase transitions involve large length scales and only certain gross features of the models are expected to matter at these length scales. Consequently a continuum or hydrodynamic description is useful. By this process, one achieves a separation of length scales, that can be exploited to identify the boundary driven phenomena. Since nonequilibrium problems are characterized by the existence of nonvanishing currents in the system, the nature of currents hold vital information about the system.

2 MODEL

In asymmetric exclusion process, particles are injected at $i = 0$ of a lattice at a rate α per unit time and withdrawn at $i = N$ at a rate $1-\gamma$ per unit time. The lattice spacing a is much smaller than the total length $Na (a \ll Na)$. The particles hop unidirectionally to the right only if the next site is unoccupied or empty. This is the hard core repulsion (exclusion) of the particles. The injection and the withdrawal of the particles act as the drive that forces a current from left to right. This hopping process conserves the particle number along the track. In addition to the hopping, one may allow particle exchange with the surrounding. A particle can be absorbed at a site at a rate ω_a if it is vacant while an occupied site may lose a particle (desorption) at a rate ω_d. These processes do not conserve particle number on the track. In absence of hopping, the evaporation/deposition process would like to maintain an average density at each site without any current along the track. This is therefore an equilibrium like situation (Langmuir kinetics) that tries to maintain a homogeneous density $\omega_a/(\omega_a+\omega_d)$. The competition of the conserved and nonconserved processes leads to inhomogeneity in the density profile and occasionally discontinuities in the density ("shocks").

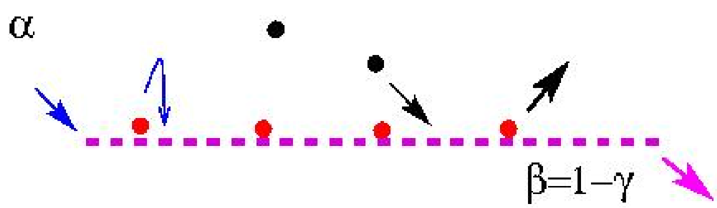

Figure 1: The model:

The possible steady states are shown in the phase diagram of the two external parameters α and γ in Fig. 2. In the low α region, the bulk density profile is determined by the injection rate and is to be called the α-phase (also called the low density phase) while for large α, the bulk density is controlled by the withdrawal rate. This phase is to be called the γ-phase. Inbetween there is a phase where the injection rate and the withdrawal rates control their own territories, meeting at a point with a discontinuity (or a "shock"). This phase is the shock phase.
The phase diagram for the conserved case shows three phases, the α-, the γ- and a maximal current phase (a dream of any traffic engineer). Nonconservation not only kills this maximal current phase but instead introduces a shock phase (traffic jam - a nightmare).
We adopt an equilibrium like definition that if the density shows a jump in going from one phase to the other, it is a first order transition, but if it changes continuously then it is a continuous or critical transition. The α- to the shock phase transition is first order because the shock height is finite on the phase boundary. However, the shock height vanishes at a particular point (α_c, γ_c). If α is changed at a fixed $\gamma = \gamma_c$, then on crossing the phase boundary, the shock height increases from zero as one enters the shock phase. This, by definition, is a critical point which does not occur in the conserved case. For $\gamma < \gamma_c$, the phase boundary is accidentally a continuation of the critical point. The shock to the γ-phase is also first order without any critical point. In this paper we concentrate on the phase boundary for the α-phase to the shock phase, especially in the neighbourhood of the critical point.

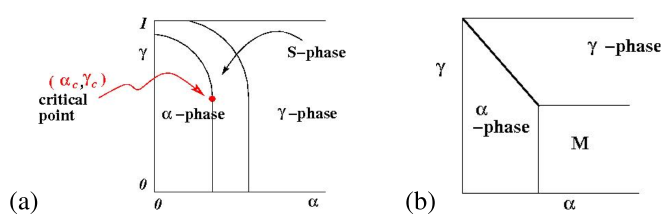

Figure 2: The phase diagrams for the nonconserved (a) and the conserved (b) model.

The density profiles in the three phases of the nonconserved case are shown schematically in Fig. 3. The point to note in these diagrams is the behaviour near the boundary. These are the boundary layers on which we would focus in this paper.

2.1 Exponents

The critical point has a few characteristic exponents. E.g.,

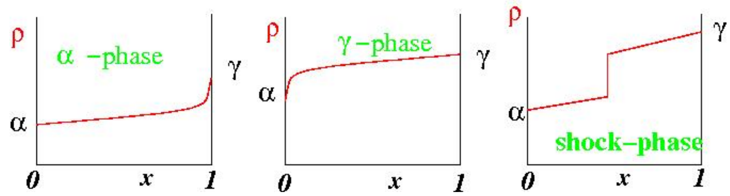

Figure 3: The density profile for the three phases of the nonconserved case.

- The shape of the phase boundary near the critical point is given by

$$\mid \gamma - \gamma_c \mid \sim \mid \alpha - \alpha_c \mid^{\chi} . \tag{1}$$

- The shock height h goes to zero along the phase boundary as

$$h \sim \mathsf{s}^{\beta}, \tag{2}$$

where s measures the deviation from the critical point along the phase boundary. For the type of phase boundary shown in Fig. 2a, s can be taken as $\Delta\gamma \equiv \gamma - \gamma_c$.

- In the shock phase the location of the shock is in the bulk of the system. As one approaches the phase boundary within the shock phase, the location x_s of the shock should approach the boundary $x = 1$, as

$$1 - x_s \sim \mid \alpha - \alpha_c \mid^{\zeta} . \tag{3}$$

- Within the shock phase if one approaches the critical point along $\gamma = \gamma_c$, the shock height vanishes as

$$h \sim \mid \alpha - \alpha_c \mid^{\overline{\beta}} . \tag{4}$$

These exponents are determined by the boundary behaviour and the boundary layer itself is characterized by two exponents, one describing its intrinsic width w and the other one its location ξ from the boundary. The location ξ is a measure of the thickness of the layer. The width w diverges at the critical point but the thickness ξ diverges as the shock is formed from the α-phase or the γ-phase side. The divergence of ξ is associated with the "shockening" transition to be explained below. The exponents describing these boundary effects are

$$\xi \sim \mid \alpha - \alpha_s \mid^{-\zeta_-}, \qquad \text{for } \alpha \to \alpha(\gamma)-, \gamma \neq \gamma_c \tag{5}$$

$$w \sim \mid \alpha - \alpha_c \mid^{-\zeta_c}, \qquad \text{for } \alpha \to \alpha_c - \text{ with } \gamma = \gamma_c. \tag{6}$$

Note that the boundary characteristic exponent ζ_- is the analog of the bulk exponent ζ of Eq. (3).
Since the bulk and the boundary transitions are linked, one needs exponents that couple them. One of these is the relation between w and h. On the first phase boundary,

$$w \sim h^{-\eta}, \tag{7}$$

which connects the divergence of w at the critical point with the vanishing of the shock height.

The microscopic variables are the occupation numbers $t_i = 0, 1$ of the ith site with 0 denoting unoccupied and 1 denoting occupied sites. In a coarse grained description and in the continuum limit, we replace these microscopic variable by the average occupation number or density $\rho(x)$ where $x = i/N$ is the position variable in the range $[0, 1]$. This continuum limit is valid for $Na \gg a$ (a being the lattice spacing). In our approach $\epsilon = 1/N$ is a small parameter.
In the steady state the spatially average density is

$$M = \int_0^1 \rho(x)dx \tag{8}$$

This can be used to define response functions that monitor sensitivity to the external drives, namely,

$$\chi_\mu = \frac{\partial M}{\partial \mu}, \quad \mu = \alpha \text{ or } \gamma. \tag{9}$$

For example, for the α-phase, $\chi_\alpha \sim O(1)$ but $\chi_\gamma = 0$. Both are nonzero for the shock phase. Thus χ_μ can be used to identify phases.
In the continuum limit, the variation of the density can be written as a modified continuity equation,

$$\frac{\partial \rho(x)}{\partial t} + \frac{\partial J_0(x,t)}{\partial x} = S_0(\rho, t), \tag{10}$$

where $J_0(x,t)$ is the current through the track and S_0 is the nonconserved current. For the simple uncorrelated Langmuir dynamics we are considering,

$$S_0 = \Omega(\rho_L - \rho), \text{ where } \rho_L = \frac{\omega_a}{\omega_a + \omega_d}, \; \Omega = N(\omega_a + \omega_d). \tag{11}$$

The nonconserved processes matter if the total flux Ω is comparable to the current and so Ω is taken to be $O(1)$ in the limit $N \to \infty$. We take $\rho_L \neq 1/2$ or $\omega_a \neq \omega_d$.
The current in the mean field approximation is taken to be determined by the local density so that it can be written as

$$J_0 = -\epsilon \frac{\partial \rho}{\partial x} + j(\rho(x,t)), \tag{12}$$

where j is the bulk current. There is an extra term reminiscent of Fick's law but with vanishingly small diffusion constant $\epsilon = 1/N$. This small diffusion constant plays an important role in determining the phase transitions. The form of $j(\rho)$ is known for several cases. In case there is a particle-hole symmetry, the simplest form is $j = \rho(1 - \rho)$. A double-peaked current density is also known to occur in an interacting system. With the form of current in Eq. 12, the equation governing the density is of the form

$$-\epsilon \frac{d^2\rho}{dx^2} + S_1(\rho)\frac{d\rho}{dx} + S_0(\rho) = 0, \text{where } S_1(\rho) = \frac{dj(\rho)}{d\rho}. \tag{13}$$

A simple expressino like $j(\rho) = \rho(1-\rho)$ quite often helps to check the general results and suffices for the simple ASEP model we have defined. More complicated form will be introduced below. $S_1(\rho)$ is zero at the peak of the current, or the density at which current is maximum.
Eq. 13 entails two length scales, (i) x for the bulk and (ii) $\tilde{x} = (x - x_0)/\epsilon$ which is significant only in a thin region as $\epsilon \to 0$ around an appropriately chosen x_0. Eq.

13 does not depend on the choice of x_0. The separation of the two scales is used to develop a uniform approximation of the solution order by order in ϵ. Here we restrict ourselves to the lowest order approximant.

The bulk solution in terms of x comes from the first order equation obtained with $\epsilon = 0$ in Eq. 13. This solution, to be called the outer solution,

$$\rho(x) = \rho_{\rm out}(x) \tag{14}$$

is given implicitly by

$$g(\rho) = 2\Omega\, x + C, \tag{15}$$

where C is a constant to be fixed by only one of the two boundary conditions.

For the left boundary condition, the outer solution is

$$g(\rho) = 2\Omega\, x + g(\alpha), \tag{16}$$

with a density

$$\rho_o \equiv \rho_{\rm out}(1) \text{ at } x = 1, \tag{17}$$

determined by

$$g(\rho_o) = 2\Omega + g(\alpha). \tag{18}$$

In general $\rho_o \neq \gamma$. To satisfy this other boundary condition $\rho = \gamma$ at $x = 1$, we use the second scale $\tilde{x} = (x-1)/\epsilon$ around the boundary point $x = 1$. With this variable, the density (to be called the inner solution) satisfies

$$-\frac{d^2\rho_{\rm in}}{d\tilde{x}^2} + S_1(\rho_{\rm in})\frac{d\rho_{\rm in}}{d\tilde{x}} = 0, \tag{19}$$

obtained from Eq. (9) by first changing the variable to $\tilde{x}$ and then taking $\epsilon \to 0$. The absence of the S_0 term can be understood from the observation that for a constant Ω this layer is too thin for the nonconservation to matter, at least to leading order in ϵ. For a smooth density profile (the solution of the second order equation), we need to match the outer and the inner solutions by requiring that

$$\lim_{x\to 1} \rho_{\rm out}(x) = \lim_{\tilde{x}\to -\infty} \rho_{\rm in}(\tilde{x}). \tag{20}$$

Here $\tilde{x} \to -\infty$ gives the outer limit of the inner solution. Incorporating this matching condition, Eq. 19 can be written as

$$\frac{d\rho_{\rm in}}{d\tilde{x}} = j(\rho_{\rm in}) - j(\rho_o), \tag{21}$$

in the thin boundary layer, with $\rho_{\rm in}(\tilde{x} = 0) = \gamma$. The complete matched solution is obtained by joining the inner and outer approximations and subtracting their common value. Therefore, the density profile is given by

$$\rho(x) = \rho_{\rm out}(x) - \rho_o + \rho_{\rm in}(\tilde{x}) + O(\epsilon). \tag{22}$$

Eq. 22 identifies the scale dependent separation of the bulk and the boundary contributions and it provides a uniform approximation of the density in the whole domain including the boundaries.

3.1 Shocks from Boundary layers:Shockening transition

A shock is formed if the inner solution fails to satisfy the boundary condition $\rho(x=1)=\gamma$. If the inner solution saturates to a density ρ_s as $\tilde{x}\to\infty$ then Eq.21 can also be written as

$$\frac{d\rho_{\rm in}}{d\tilde{x}} = -(\rho-\rho_{\rm o})(\rho-\rho_{\rm s})\Phi(\rho) \tag{23}$$

where one zero of the function at $\rho_{\rm o}$ corresponds to the matching condition and the other one for the saturation. The inner solution is of the form

$$\rho_{\rm in}(\tilde{x}) = \mathcal{I}(\tilde{x}/w+\xi) \text{ with } \mathcal{I}(z)\to\rho_s \text{ or } \rho_{\rm o} \text{ as } z\to\pm\infty. \tag{24}$$

Here w is the width of the layer and ξ gives the location of the center of the layer - the two quantities defined in Eqs. (5) and 6. Even if ξ is outside the physical range it helps in visualization of the shock formation. This form gives a direct interpretation of the width w but one may also define w from the approach of the inner density to the bulk asymptote in the outer region.

There are two types of solutions for the inner density(4), one bounded between ρ_o and ρ_s while the other one shows a divergence with $d\rho/dx\sim-\rho^2$, or more generally, $d\rho/dx\sim-\rho^{2p}$. It transpires that for the class of unbounded solution it is always possible to match the boundary condition by suitably shifting the center of the inner solution. This will not be the case for the bounded solution. The significance of this is that the bounded solution can give rise to shocks but not the unbounded ones.

For a given α, as γ is changed, two different situations may arise; the origin or the center of the layer shifts either to $-\infty$ ($\xi\to-\infty$) or to +infinity, $\xi\to+\infty$.

In the first situation, the boundary layer as seen in the physical range thickens but remaining pinned to the boundary. As $\xi\to-\infty$ (note this is the inner scale), the layer gets released from the boundary and moves into the bulk. The transition of a thin layer to a shock at $\gamma=\rho_s(\alpha)$ has been called a "shockening" transition(3). So long as the boundary layer stays pinned to the boundary, $\chi_\gamma\sim\epsilon\gamma/\hat{S}_1(\gamma)\to0$ as $\epsilon\to0$. In contrast, χ_α is nonzero. The phase, by definition, is then an α-phase. The bulk shock phase boundary is given by $\gamma=\rho_s(\alpha)$.

The occurrence of the two zeros of $\hat{S}_1(\rho)$ in Eq. 23 suggests that there has to be another line $\gamma=\rho_{\rm o}(\alpha)$ at which $\xi\to+\infty$. We call this the Mukherji-Mishra (MM) dual boundary line because a similar feature was observed in Ref. (4). As one crosses this MM line the boundary region goes from an accumulated to a depleted region, thereby separating the shockening to nonshockening boundary layers. This MM dual line is purely a boundary transition line, and its existence is a requirement for shock formation at $\gamma=\rho_{\rm s}(\alpha)$. Since $(\rho_{\rm o},\rho_{\rm s})$ need to occur in pair, we call the $\gamma=\rho_{\rm o}(\alpha)$ as the dual line of the bulk phase boundary.

Once we know the bulk phase boundary and the dual line, we can obtain the width of the layer. From the asymptotic approach to the limits ρ_o and ρ_s, one gets from Eq. 23, $w^{-1}=(\rho_s-\rho_{\rm o})\Phi(\rho_X)$ with X denoting 'o' or 's'. This also shows the possibility of a critical point where w diverges. It happens if the shockening transition line and the dual line intersect. The intersection is at $\gamma=\gamma_c$ and since $\rho_{\rm o}\to\rho_{\rm s}$, we find $w\to\infty$, with $\eta=1$ (see Eq. 7). It also follows that the shock height remains nonzero at the bulk phase transition from the α-phase to the shock phase. On the other hand, the shock evolves from a zero height at the crossing point so that it is a continuous transition. In case the two lines do not cross, there will be no critical point and the lines will be symmetrically placed around $\gamma=\rho_m$, the maximum current density. The bulk phase diagram corresponds to Fig. 2.

The exponents follow from the analytical behaviour of the outer solutions $g(\rho)$. Noting that $dg(\rho)/d\rho=0$ at $\rho=\rho_c$, one gets

$$\zeta_c=1/2, \zeta_-=0(\log), \text{ and } \eta=1, \tag{25}$$

where for completeness we have included η obtained above. The notation "(log)" means a logarithmic divergence because the power law exponent is zero.

The bulk exponents also follow quite generally from a Taylor series expansion of the outer solutions without knowing the details of the outer solution. For example, the shape of the phase boundary near the critical point can be obtained by expanding $g(\rho)$ in Eq. (18) around $\rho = \gamma_c$, $x = 1$ on the left hand side and $\rho = \alpha_c$ on th left hand side. Consequently, one gets

$$\chi = 1/2,\ \beta = 1,\ \overline{\beta} = 1/3, \text{and } \zeta = 2/3. \tag{26}$$

We see that these exponents are determined purely by the analytic nature of outer densities and are therefore insensitive to the many microscopic details. It is therefore expected to be universal across models. Only certain gross symmetry properties are important in determining their values. For example the current for Fig. 2 is symmetric around $\rho = /2$. But that is not important for the exponents. The same values will be obtained for an asymmetric current also provided the peak is quadratic in nature.(5).

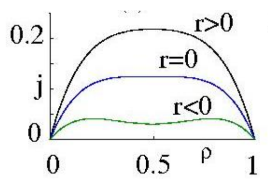

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Figure 4: Current versus ρ for three values of r. There is a double peak in the current for $r < 0$. The flatness of the top for $r = 0$ is responsible for the tricriticality.

4 Tricritical point

Let us now consider an application of the idea of duality in a problem with interaction that can show symmetry breaking in the phase diagram and how one gets a tricritical point(9). The particles hop to the right with mutual exclusion as before so that the occupation number at a site is 0 or 1. In addition, there is a next nearest neighbour repulsion(6) so that

$$\begin{array}{lcll} 1100 & \rightarrow & 1010 & \text{with a rate } 1+\varepsilon, \\ 0101 & \rightarrow & 0011 & \text{at a rate} 1-\varepsilon, \end{array}$$

with ($0 < \varepsilon < 1$) (not to be confused with the small parameter ϵ).
The exactly known stationary current(6) for the conserved system shows the change from single to double peak for ε close to $\varepsilon = \varepsilon_{\rm J} \approx 0.8$. This model is known to show many features including double shocks(7; 8). To simplify the problem, one may do a Taylor series expansion in ρ and ε of the exactly known current upto fourth order. For simplicity we work with this expansion in a general form

$$j(\rho) = \frac{2r+u}{16} - \frac{r}{2}(\rho - \frac{1}{2})^2 - u\,(\rho - \frac{1}{2})^4, \tag{27}$$

with the constant piece chosen to ensure that the current vanishes for $\rho = 0, 1$ (the empty track and the fully-occupied track). Eq. 27 for $r = 2, u = 0$ recovers the known current density for ASEP processes ($j = (1-\rho)\rho$) while the double peak appears for $r < 0$. Throughout u is taken as a positive constant, and r is tunable but kept small. The current is shown in Fig. 4a for typical values of r.
For $r > 0$, with a single peak in the current, the duality argument shows that the critical point will have $\gamma_c = 1/2$, but α_c depending on r. The shape of the transition curve near the critical point is the same as in the previous section.

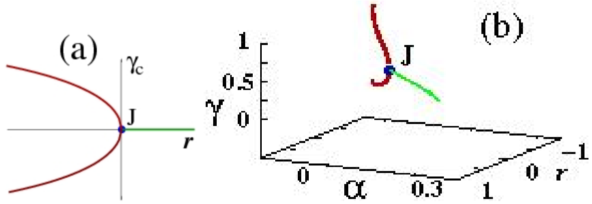

Figure 5: (a) The critical lines in the γ-r plane, where $r = \varepsilon - \varepsilon_J$. The width vanishes with a characteristic exponent as $r \to 0-$. (b) Three dimensional view of the tricritical point J in the α-γ-r space. Only the critical lines are shown. These lines are noplanar and (a) shows the projection.

For $r \leq 0$, the situation is different. For negative r, there is the possibility of two critical points corresponding to γ taking the values of the peak densities. Near the peak, the current is quadratic in the density deviation as in the case studied in Sec. 2. There will therefore be two critical points each with the same set of exponents as in the single peak case. They are in the same universality class.
If the parameter r is tuned, the phase diagram can be drawn in a three dimensional space $\alpha - \gamma - r$. For positive r, the locus of the critical point is a line, every point of which has the same set of exponents. This line undergoes a bifurcation into two lines for $r < 0$ as shown in Fig. 5a. There is no change in the critical exponents along the two lines. These lines are shown in Fig. 5b in the three parameter space. The special case is the bifurcation point, the special point J. This is the tricritical point.
The tricritical point J, being at the intersection of the shock line and the dual line, is at

$$g_{r=0}(\gamma_{\rm J}) = 2\Omega + g_{r=0}(\alpha_{\rm J}), \quad \gamma_{\rm J} = 1/2. \tag{28}$$

Since $S_1(\rho) \sim (\rho - 1/2)^3$, the shape exponent is

$$\chi_{\rm J} = 1/4, \tag{29}$$

where $\chi_{\rm J}$ is defined as

$$\gamma - \gamma_{\rm J} \sim \mid \alpha - \alpha_{\rm J} \mid^{\chi_{\rm J}} . \tag{30}$$

More details on this nonequilibrium tricritical point can be found in Ref. (9). We point out here that the first order transition lines of Fig 2a become surfaces in the three dimensional phase diagram. These first-order surfaces end on critical lines shown in Fig. 5b.

4.1 Conclusions

We discussed the role of boundary layers in nonequilibrium phase transitions in models where the bulk transition is driven by the boundary. The resulting bulk phase diagrams can be qualitatively and quantitatively understood via the shockening transition, a process of deconfinement of the boundary layer. The shockening transition that induces a bulk phase transition has a dual boundary transition and the intersection of the two gives a critical point. This duality has been used to obtain and characterize a nonequilibrium tricritical point in an interacting case.

Acknowledgments
I thank Sutapa Mukherji and Jaya Maji for collaborations and many discussions.

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