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LETTER TO THE EDITOR

Nonequilibrium criticality at shock formation in steady states

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Online at stacks.iop.org/JPhysA/38/L285**Abstract**

The steady-state shock formation in processes such as nonconserving asymmetric simple exclusion processes in varied situations is shown to have a precursor of a critical deconfinement transition on the low-density side. The diverging length scales and the quantitative description of the transition are obtained from a few general properties of the dynamics without relying on specific details.

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Asymmetric simple exclusion processes (ASEP) involve particles hopping in a preferred direction under hard-core repulsion that forbids double occupancy on a site [1]. This model with periodic [2, 3] and open boundary conditions [4] as well as its variants involving different update schemes [5] have been extensively studied in order to gain general understanding of far-from-equilibrium processes. In addition to this, ASEP has a direct resemblance with the transport processes within the cell, provided the dynamics of ASEP is modified by allowing attachment and detachment of particles from or to the environment respectively. The motor proteins which participate in cellular transportation by moving on linear tracks laid by long bio-molecules play the role of particles in ASEP [6–9].

In the presence of open boundaries, one needs to think of two particle reservoirs attached to the boundaries which either inject or withdraw particles to or from the boundaries with certain specified rates. An additional reservoir is needed for the desorption/adsorption kinetics (Langmuir kinetics) of particles on the lattice. The biased hopping of the particles, injected at one end by the reservoir, causes a finite current in the system even in the steady state. It is intuitively understandable that this particle current would help in the propagation of the boundary information to the bulk of the system. Thus, unlike equilibrium systems, here boundaries play a crucial role in the steady-state dynamics and can give rise to several new features such as boundary-driven phase transition or production of shocks in the density profile [10, 11].

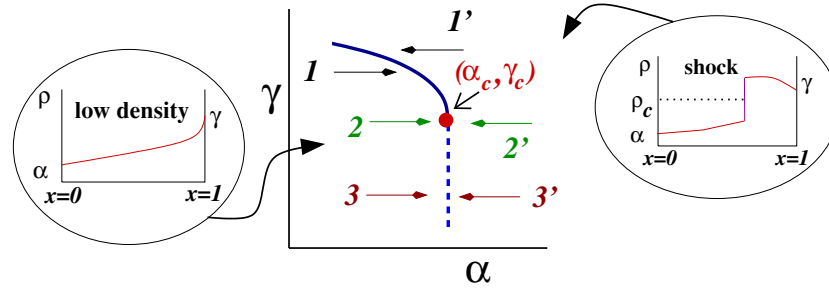


Figure 1. Bulk phase boundary in the $\alpha - \gamma$ plane, separating a low-density phase and a phase with a shock (insets show the density variation ρ versus x). The critical point is at (α_c, γ_c) . The shock has a nonzero height on the solid line of the phase boundary, $\gamma > \gamma_c$ but the height vanishes on the dashed part, $\gamma < \gamma_c$. Arrows indicate various paths used in the text.

(This figure is in colour only in the electronic version)

The boundary-related event, which concerns us here, is the appearance of localized shocks in the density profile. Various aspects of shocks, which are discontinuities in the particle density profile over a microscopic distance in the bulk, have been extensively studied in the past. If α and γ are the densities maintained by the reservoirs at the two ends, then in the (α, γ) plane there are lines $\alpha = \alpha_s(\gamma)$ demarcating the possible phases (see figure 1). Such bulk phase diagrams are now known for many cases and in fact mean-field descriptions seem to give a good description of the bulk phase diagrams, especially for the shock formation [7, 10, 12, 13]. Here we show the existence of a novel deconfinement transition of a layer near an open end as the phase boundary is approached from the low-density side, reminiscent of the equilibrium wetting transition [14]. This layer with a non-bulk density profile remains attached to the end point but, after deconfinement, admits the bulk density variation though with a shock. Let us call this special layer a shockening layer and the transition a *shockening* transition.

The shockening transition on the low-density side is a precursor to the bulk phase transition, and shows power-law behaviours. This criticality is characterized by two length scales ξ and w , where $\xi \rightarrow \infty$ leads to deconfinement while w gives the length scale for the crossover of the surface density profile to the bulk. Though w in general remains finite, there is a possibility of $w \rightarrow \infty$ which would signal a criticality at (α_c, γ_c) on the bulk phase transition line. These divergences are described by the exponents ζ_- and ζ_c defined by

$$\xi \sim |\Delta\alpha|^{-\zeta_-}, \quad \text{for } \Delta\alpha \equiv \alpha - \alpha_s(\gamma) \rightarrow 0-, \quad (1)$$

$$w \sim |\Delta\alpha|^{-\zeta_c}, \quad \text{for } \Delta\alpha \equiv \alpha - \alpha_c \rightarrow 0-, \quad (2)$$

where $\Delta\alpha$ measures the deviation from the phase boundary for a fixed γ . In equation (1), it is along a path like path 1 in figure 1 with $\gamma \neq \gamma_c$ while for equation (2) it is for $\gamma = \gamma_c$ (path 2 in figure 1). By analysing a general equation for the steady state, we show that these two exponents ζ_- and ζ_c (and, in fact, several other bulk exponents defined below) are *universal* as they are determined by only a few general properties of the dynamics and not in detail.

A very well-studied example is the case of nonconserving ASEP of one species on a lattice of N sites. The particles can jump to the neighbouring forward site if it is empty. Apart from that, the bulk of the system is attached to a particle reservoir such that a particle can attach to (detach from) the chain with a rate ω_a (ω_d). The dynamics at the left boundary is that of the injection of particles with a rate α while at the right it is withdrawal at the rate $1 - \gamma$. Since

the mean-field dynamics through average density like variables gives a good description of the bulk phase diagram, we adopt the same approach to study the shockening transition. This is expected to capture the overall features of the transition though fluctuations may affect the exponents. The role of fluctuations will be studied elsewhere.

The mean-field equation, describing the evolution of the particle density at a site i , is expressed in terms of the density $n_i = \langle \tau_i \rangle$, where τ_i is the occupation number of site i , and $\langle \dots \rangle$ denotes statistical average. The dynamics is given by

$$\frac{dn_i}{dt} = n_{i-1}(1 - n_i) - n_i(1 - n_{i+1}) + \omega_a(1 - n_i) - \omega_d n_i. \quad (3)$$

This dynamics can obviously be extended to incorporate other effects as well. In the large- N limit, a continuum mean-field approach is based on the density variable $\rho(x)$ related to τ as $\langle \tau_{i\pm 1} \rangle = \rho(x) \pm \frac{1}{N} \frac{\partial \rho}{\partial x} + \frac{1}{2N^2} \frac{\partial^2 \rho}{\partial x^2} \dots$ treating $1/N$ as the lattice spacing with x in the range $[0, 1]$. The various forms of single species dynamics studied so far can be written in a general form (for the steady state)

$$\epsilon \frac{d}{dx} f_2(\rho) \frac{d\rho}{dx} + f_1(\rho) \frac{d\rho}{dx} + \Omega f_0(\rho) = 0, \quad (4)$$

with $f_i(\rho)$, $i = 0, 1, 2$, specifying the dynamics of the system and $\Omega = \omega_d N$. The steady-state density profile satisfies the two-boundary conditions $\rho(x = 0) = \alpha$ and $\rho(x = 1) = \gamma$ at the two ends. Here $\epsilon \equiv (2N)^{-1}$ is the small parameter. For example, for the case of noninteracting particles in equation (3) the f -functions of equation (4) are

$$f_2(\rho) = 1, \quad f_1(\rho) = 2\rho - 1, \quad f_0(\rho) = K(1 - \rho) - \rho, \quad (K = \omega_a/\omega_d). \quad (5)$$

The complexity of the functions f_i increases with the interaction and other details but explicit knowledge of these functions is not essential for the analysis reported here.

The dynamics of equation (4) admits two special densities. (i) The Langmuir density corresponding to $\rho = \rho_L$ at which $f_0(\rho_L) = 0$; $\rho(x) = \rho_L$ is a particular solution of equation (4). It represents the steady-state bulk density if adsorption/desorption were the sole dynamics in the problem. (ii) A density $\rho = \rho_c$ at which $f_1(\rho) = 0$. In the case of a simple zero, for small deviation $\rho = \rho_c + \delta\rho$, the hopping rules show a special symmetry of invariance of the first derivative term under $\delta\rho \rightarrow -\delta\rho$. This is the particle-hole symmetry of equation (5). The bulk dynamics may not respect this symmetry in the general case of $\rho_c \neq \rho_L$. The special symmetry occurs for $\rho_c = \rho_L$ as e.g. for equation (5) when $K = 1$. We take $f_2(\rho) \neq 0$ for $0 \leq \rho \leq 1$. The cases of non-simple zeros or zeros of $f_2(\rho)$ are to be discussed elsewhere.

To study the shockening transition, we generate a uniform approximation of the solution of equation (4) via a leading-order boundary layer analysis [15]. In general both the boundary conditions cannot be satisfied if the second derivative term ($\epsilon \rightarrow 0$) is ignored. As a result there appears a boundary layer at one end or a shock somewhere in the interior (or both). Within this special region, the second derivative term is needed. By neglecting appropriate terms from the original equation, one obtains two different solutions, to be called the outer and the inner solutions such that the outer solution is valid over almost the entire system and the inner solution is valid only in the region where the boundary layer or the shock appears. The two solutions join smoothly. As a general rule, if the inner solution attains a saturation then the boundary condition might not be satisfied by the inner solution. This is the criterion for shock formation. In this situation, the two-boundary conditions are satisfied by two different outer solutions connected by the inner solution in the interior forming a shock layer.

Without loss of generality we choose the boundary or shock layer to be at or near $x = 1$. For equation (4) the outer and inner solutions come from

$$\frac{d\rho_{\text{out}}}{dx} = -\Omega \frac{f_0(\rho_{\text{out}})}{f_1(\rho_{\text{out}})}, \quad \text{and} \quad \frac{d\rho_{\text{in}}}{d\tilde{x}} = \frac{F(\rho_{\text{in}})}{f_2(\rho_{\text{in}})}, \quad (6)$$

where $\tilde{x} = (x - x_d)/\epsilon$ is the inner variable, x_d giving the location of the layer or the shock, and

$$F(\rho) \equiv \hat{f}_1(\rho_o) - \hat{f}_1(\rho), \quad \text{with} \quad \frac{d\hat{f}_1(\rho)}{d\rho} = f_1(\rho). \quad (7)$$

The matching condition $\rho_{\text{in}}(\tilde{x} \rightarrow -\infty) = \rho_o \equiv \rho_{\text{out}}(1)$, for smooth joining has been incorporated in equation (7).

Given that $\rho(0) = \alpha$ the relevant inner and outer solutions are

$$\rho_{\text{in}}(\tilde{x}) = \rho_o S_{\text{in}}(\tilde{x}/w + \xi), \quad \text{and} \quad \Omega x = g(\rho_{\text{out}}) - g(\alpha) \quad (\text{left solution}) \quad (8)$$

with $S_{\text{in}}(\tilde{x}) \rightarrow 1$ as $\tilde{x} \rightarrow -\infty$. The functional forms of $g(\rho)$ and $S_{\text{in}}(\tilde{x})$ depend on the details of f -functions. By choosing the shift $x_d = 1$, ξ is determined by

$$\rho_o S_{\text{in}}(\xi) = \gamma. \quad (9)$$

For example for equation (5),

$$g(\rho) = \frac{1}{1+K} \left(2\rho + \frac{K-1}{1+K} \log[K - (1+K)\rho] \right), \quad (10)$$

and $S_{\text{in}}(\tilde{x}) \sim \tanh(\tilde{x}/(2w) + \xi)$, for all K . The two scales mentioned in equations (1) and (2) appear in the inner solution. There is an N -dependence of $\xi \sim N^{-\nu_-}$ with an exponent $\nu_- = 1$ to make ξ act also as the finite size scaling variable for the transition.

The condition for saturation of $S_{\text{in}}(\tilde{x})$ is

$$F(\rho) = 0 \quad \text{for} \quad \rho = \rho_s > \rho_o. \quad (11)$$

For $\gamma > \rho_{\text{in}}(\tilde{x} \rightarrow \infty)$ the boundary condition cannot be satisfied by ρ_{in} leading to shock formation. Therefore the phase boundary is given by $\gamma = \rho_s(\rho_o(\alpha_s))$ with shocks appearing for $\alpha > \alpha_s(\gamma)$. We note here that since $F(\rho)$ has a vanishing derivative at $\rho = \rho_c$, by Rolle's theorem of calculus, $\rho_o \leq \rho_c \leq \rho_s$. In the phase with shock, the centre of the shock can always be chosen such that $\rho_{\text{in}}(0) = \rho_c$ at $x_d = x_s$.

Assuming simple zeros at $\rho = \rho_o$ and $\rho = \rho_s$, we write

$$F(\rho) = -(\rho - \rho_o)(\rho - \rho_s)\phi(\rho), \quad (12)$$

which defines $\phi(\rho)$. For the case of equation (5), $\phi(\rho) = 1$. The large \tilde{x} behaviour is then given by

$$\frac{d\rho}{d\tilde{x}} \approx -\frac{\rho - \rho_s}{w(\alpha)}, \quad \text{where} \quad w(\alpha) = (\rho_s - \rho_o)^{-1} \frac{f_2(\rho_s)}{\phi(\rho_s)}, \quad (13)$$

with w depending only on α and not on γ . Equation (13) shows $w(\alpha)$ as the characteristic length scale for approach to saturation or the bulk density, as defined earlier. A similar equation describes the approach to ρ_o with a scale $w_0 \propto w$. This allows a practical definition of w as

$$w^{-1} = -d \ln(\rho(x) - \rho_{\text{out}}(x))/d\tilde{x}|_{\tilde{x} \rightarrow -\infty}, \quad (14)$$

noting that $\rho_{\text{out}}(x)$ is the bulk density and the deviation is only in the boundary layer region.

The behaviour of ξ near the phase boundary, for a fixed γ , can be determined from the condition at $\tilde{x} = 0$, equation (9). For γ greater than but close to γ_c , equation (6) together with equation (12), yield

$$\xi \sim \ln|\gamma - \rho_s| \sim \ln|\Delta\alpha|, \quad \text{or} \quad \zeta_- = 0(\log), \quad (15)$$

from equation (1). This scale ξ depends on both the boundary conditions. It should be noted that the shockening transition from the low-density side determines the phase boundary.

For a given γ , w may be made to diverge by tuning α . This locates the critical point on the phase boundary at (α_c, γ_c) such that

$$g(\gamma_c) - g(\alpha_c) = \Omega, \quad \text{with } \rho_o = \rho_s = \rho_c = \gamma_c. \tag{16}$$

If the boundary condition at $x = 1$ is held fixed at $\gamma = \gamma_c$, then for $\alpha \rightarrow \alpha_c$, both ρ_o and ρ_s approach ρ_c . For $\rho_o = \rho_c - \delta\rho$ and $\alpha = \alpha_c - \delta\alpha$ one may expand equation (8) in $\delta\rho, \delta\alpha$ with $x = 1$. Now, by definition, $g'(\rho) = f_1(\rho)/f_0(\rho)$, so that

$$g'(\rho_c) = 0, \quad \text{if } \rho_c \neq \rho_L. \tag{17}$$

We therefore have $w \sim |\rho_s - \rho_o|^{-1} \sim |\Delta\alpha|^{-\zeta_c}$, where

$$\zeta_c = 1/2, \quad \text{if } \rho_c \neq \rho_L, \quad \text{but } \zeta_c = 1, \quad \text{if } \rho_c = \rho_L. \tag{18}$$

The density for the critical point also shows a singular variation near the end point, namely, $\rho_c - \rho(x) \sim \sqrt{1-x}$ for $x \rightarrow 1-$, if $\rho_c \neq \rho_L$. This follows from equation (6) as a consequence of the simple zero of $f_1(\rho)$. These results can be verified for the special case of equation (5) but are seen here to be of more general validity.

The shape of the phase boundary can be determined in a similar way. For $\gamma = \gamma_c + \Delta\gamma$, equation (8), with $x = 1$, on expansion gives

$$-g'(\rho_c)\Delta\gamma + g''(\rho_c)(\Delta\gamma)^2/2 + \dots = g'(\alpha_c)\Delta\alpha \dots$$

The phase boundary therefore takes the form $\Delta\gamma \sim |\Delta\alpha|^{\chi_-}$ with

$$\chi_- = 1, \quad \text{if } g'(\rho_c) \neq 0 \quad (\text{e.g. } K = 1) \tag{19}$$

$$= 1/2, \quad \text{if } g'(\rho_c) = 0, \quad (\text{e.g. } K \neq 1) \tag{20}$$

where K refers to equation (5). The analogous exponent χ_+ for $\gamma < \gamma_c$ is discussed later.

Though w measures the crossover length, right on the phase boundary, it is related to the height of the shock that forms beyond the phase boundary, namely, $h = \rho_s - \rho_o \sim w^{-1}$. The mean-field results, based on power series expansion, seem to require $\chi_- \leq 1$ so that the phase boundary is not tangential to the α -axis. This implies that $\Delta\gamma$ can be taken as a measure of distance r from the critical point measured along the phase boundary, i.e., $r \sim \Delta\gamma$. Along this curve, for $\gamma \geq \gamma_c$ or $r \leq 0$,

$$h \sim |r|^\beta \quad \text{with } \beta = 1. \tag{21}$$

For $\gamma < \gamma_c$, the length w remains infinite, i.e. the shock, if formed, is of zero height. In fact, the boundary layer that forms does not shocken (path 3 in figure 1). In this situation, there are two possibilities: either the shock height grows continuously as the phase boundary is crossed or the shock formation is suppressed. Though the former is the generic scenario, the latter situation can occur under special conditions such as e.g. the special symmetry when $\rho_c = \rho_L$.

We now show that the same properties of the f -functions also determine the behaviour in the deconfined region. The shock state, just after deconfinement, is described by the thickness of the deconfined layer measured by the distance of the shock from the boundary, Λ , and the height, h of the shock. If the deconfinement takes place at $x = 1$ and the shock position is x_s , then $\Lambda = 1 - x_s$. In addition the shock layer will have a width which we do not discuss here. The behaviour of h along the phase boundary is also of importance, especially as one approaches the critical point.

To discuss shock, we need the outer solution of equation (6) satisfying $\rho(1) = \gamma$ as

$$\Omega(1-x) = g(\gamma) - g(\rho_{\text{out}}) \quad (\text{right solution}). \tag{22}$$

Moreover, the shock close to the critical point is asymptotically symmetric with a scale $w = (\rho_s - \rho_o)^{-1} f_2(\rho_c)/\phi(\rho_c)$ as seen from equation (13). For a symmetric shock, centred

at $\rho = \rho_c$, its position x_s and height h satisfy equations (8) and (22) with $\rho_{\text{out}} = \rho_c \mp h/2$ respectively. By expanding equations (8) and (22) in h and $\Delta\alpha = \alpha - \alpha_c$ keeping $\gamma = \gamma_c$, we get (prime denoting derivatives) (path 2' in figure 1)

$$g'(\rho_c)h + \frac{1}{24}g'''(\rho_c)h^3 + \dots = -g'(\alpha_c)\Delta\alpha + \dots \quad (23)$$

A similar analysis for x_s can also be done. In the general case, $\rho_c \neq \rho_L$, if the third derivative of g is non-vanishing, equation (23) gives

$$h \sim |\Delta\alpha|^{\beta'}, \quad \text{with } \beta' = 1/3, \quad \text{and } \Lambda = 1 - x_s \sim |\Delta\alpha|^\zeta, \quad \text{with } \zeta = 2\beta'. \quad (24)$$

Equation (24) defines the bulk exponents β' and ζ for h and Λ respectively. These exponents have been found for equation (5) with $K \neq 1$ [7], but is shown here to be more general. There are other possibilities also. For example, in case all the derivatives of $g(\rho)$ vanish, no shock can exist [12], as, e.g., for $K = 1$ in equation (5). Such special cases will be discussed elsewhere. The exponents obtained in equation (24) remain the same for all $\gamma \leq \gamma_c$ (path 3' in figure 1) because in this regime the effective boundary condition is $\gamma = \gamma_c$, thanks to the formation of a nonshocking boundary layer at $x = 1$. A consequence of this is that $\chi_+ = 0$ for the shape of the phase boundary for $\gamma < \gamma_c$. For $\gamma > \gamma_c$ (path 1' in figure 1), h remains $O(1)$ on the phase boundary so that $\beta' = 0$ and $\zeta = 1$. It is tempting to suggest a scaling relation $\beta' + \zeta = 1$ throughout.

As a further example of the predictive power of this approach, we consider ASEP of interacting particles [16, 17] that destroys the particle-hole symmetry. Our aim is to show that the same physical picture remains valid quantitatively in this case also. In the interior, particles at site i move to site $i + 1$, provided it is empty, with a rate that depends on the state of sites $i - 1$ and $i + 2$ as $0100 \rightarrow 0010$ with a rate $1 + \delta$ and $1101 \rightarrow 1011$ with a rate $1 - \delta$, with all other rates remaining the same as for equation (3). For equal attachment and detachment rates ($K = 1$), the continuum mean-field equation describing the shape of the density profile is of the type equation (4) with $f_2(\rho) = 1 + \delta(1 - 2\rho)$, $f_1(\rho) = 1 - 2\rho + \delta[1 - 6\rho(1 - \rho)]$ while $f_0(\rho)$ remains same as in equation (5) with $K = 1$, i.e. with $\rho_L = 1/2$. Numerical (MATLAB) solution of the differential equation for relevant set of parameters actually shows that the shock is centred at $\rho_c = (1 + 3\delta - \sqrt{1 + 3\delta^2})/(6\delta)$, the zero of $f_1(\rho)$. In particular, $\rho_c < 1/2$. For the shockening transition, keeping γ fixed, the relevant zero, ρ_s , of $\hat{f}_1(\rho_o) - \hat{f}_1(\rho)$ is ($\sigma = 2\rho_o - 1$)

$$4\delta\rho_s = 1 + 2\delta - \delta\sigma - (1 - 2\delta^2 + 2\delta\sigma + 3\delta^2\sigma^2)^{1/2}. \quad (25)$$

The phase boundary between the low-density and the shock phase is determined by the condition $\gamma = \rho_s(\rho_o, \delta)$. The height of the shock on the phase boundary is $\gamma - \rho_o$ which vanishes at the critical point $\gamma_c = \rho_c$. It follows from these that the shock near the critical point is asymptotically symmetric. So the critical feature, especially of the shockening transition of this interacting system is similar to the general case considered above (except for $\delta = 0$). This can also be explicitly verified from detailed solutions.

In summary, we have shown the existence of universal behaviour associated with shockening transition, a precursor to the shock formation. The dynamics is described by a set of f functions as defined by equation (4). The zeros ρ_L and ρ_c of $f_0(\rho)$ and $f_1(\rho)$, respectively, are the two important densities for the steady state. The shock, when formed, is centred around $\rho = \rho_c$ which is a point of special symmetry. The generic situation corresponds to $\rho_c \neq \rho_L$. The thickening of the layer that leads to the shock (called the 'shockening layer') is described by two diverging scales, ξ and w whose critical behaviours are determined by the nature of $f_i(\rho)$ around $\rho = \rho_c$. Furthermore, our analysis and results suggest the possibility of more complex dynamics involving different symmetries, though such model systems are not yet known.

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