Bethe Ansatz Solution of the Asymmetric Exclusion Process with Open Boundaries

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We derive the Bethe ansatz equations describing the complete spectrum of the transition matrix of the partially asymmetric exclusion process with the most general open boundary conditions. For totally asymmetric diffusion we calculate the spectral gap, which characterizes the approach to stationarity at large times. We observe boundary induced crossovers in and between massive, diffusive and KPZ scaling regimes.

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The partially asymmetric simple exclusion process (PASEP) describes the asymmetric diffusion of particles along a one-dimensional chain with L sites. It is one of the most studied models of non-equilibrium statistical mechanics, see [1, 2] for recent reviews. This is in part due to the fact that is one of the simplest lattice gas models, but also because of its applicability to molecular diffusion in zeolites [3], bioploymers [4], traffic flow [5] and other one-dimensional complex systems [6].

At large times the PASEP exhibits a relaxation towards a nonequilibrium stationary state. An interesting feature of the PASEP is the presence of boundary induced phase transitions [7]. In particular, in an open system with two boundaries at which particles are injected and extracted with given rates, the bulk behaviour in the stationary state is strongly dependent on the injection and extraction rates. Over the last decade many stationary state properties of the PASEP with open boundaries have been determined exactly [1, 2, 8–11]. On the other hand, much less is known about its dynamics. This is in contrast to the PASEP on a ring for which exact results using Bethe's ansatz have been available for a long time [12, 13]. For open boundaries there have been several studies of dynamical properties based mainly on numerical and phenomenological methods [14, 15]. In this Letter we employ Bethe's ansatz to obtain exact results for the approach to stationarity at large times in the PASEP with open boundaries. Upon varying the boundary rates, we find crossovers in massive regions, with dynamic exponents $z = 0$, and between massive and scaling regions with diffusive ($z = 2$) and KPZ ($z = 3/2$) behaviour.

The dynamical rules of the PASEP are as follows. At any given time t each site is either occupied by a particle or empty and the system evolves subject to the following rules. In the bulk of the system ($i = 2, \ldots, L-1$) a particle attempts to hop one site to the right with rate p and one site to the left with rate q. The hop is executed unless the neighbouring site is occupied, in which case nothing happens. On the first and last sites these rules are modified. If site $i = 1$ is empty, a particle may enter the system with rate α. If on the other hand site 1 is occupied by a particle, the latter will leave the system with rate γ. Similarly, at $i = L$ particles are injected and extracted with rates δ and β respectively. With every site i we associate a Boolean variable τ_i, indicating whether a particle is present ($\tau_i = 1$) or not ($\tau_i = 0$). The state of the system at time t is then characterized by the probability distribution $P_t(\tau_1, \ldots, \tau_L)$. The time evolution of P_t occurs according to the aforementioned rules and as a result is subject to the master equation

$$\frac{\mathrm{d}P_t}{\mathrm{d}t} = MP_t. \tag{1}$$

Here M is the PASEP transition matrix whose eigenvalues have non-positive real parts. The large time behaviour of the PASEP is dominated by the eigenstates of M with the largest real parts of the corresponding eigenvalues.

Bethe's Ansatz: It is well known that the transition matrix M is related to the Hamiltonian H of the open spin-1/2 XXZ quantum spin chain through a similarity transformation $M = -\sqrt{pq}\, U_\lambda H U_\lambda^{-1}$ where H is given by [10]

$$\begin{aligned} H \;=\; -\frac{1}{2}\sum_{j=1}^{L-1} \big[\sigma_j^{\mathrm{x}}\sigma_{j+1}^{\mathrm{x}} + \sigma_j^{\mathrm{y}}\sigma_{j+1}^{\mathrm{y}} - \Delta\sigma_j^{\mathrm{z}}\sigma_{j+1}^{\mathrm{z}} \\ + h(\sigma_{j+1}^{\mathrm{z}} - \sigma_j^{\mathrm{z}}) + \Delta\big] + B_1 + B_L. \end{aligned} \tag{2}$$

The parameters Δ and h, and the boundary terms $B_{1,L}$ are related to the PASEP transition rates by

$$\begin{aligned} \Delta &= -\frac{1}{2}(Q + Q^{-1}), \quad h = \frac{1}{2}(Q - Q^{-1}), \quad Q = \sqrt{\frac{q}{p}}, \\ B_L &= \frac{\beta + \delta - (\beta-\delta)\sigma_L^{\mathrm{z}} - \frac{2\beta}{\lambda Q^{L-1}}\sigma_L^{+} - 2\delta\lambda Q^{L-1}\sigma_L^{-}}{2\sqrt{pq}}, \\ B_1 &= \frac{\alpha + \gamma + (\alpha-\gamma)\sigma_1^{\mathrm{z}} - 2\alpha\lambda\sigma_1^{-} - \frac{2\gamma}{\lambda}\sigma_1^{+}}{2\sqrt{pq}}. \end{aligned} \tag{3}$$

Here λ is a free parameter on which the spectrum does not depend and $\sigma_j^{\pm} = (\sigma_j^{\mathrm{x}} \pm \mathrm{i}\sigma_j^{\mathrm{y}})/2$.

Although it has been known for a long time that H is integrable [16], the off-diagonal terms in B_1 and B_L have presented great difficulties in diagonalizing H using e.g. Bethe's ansatz. However, recently a breakthrough was achieved [17] in the case where the parameters satisfy a constraint, which in our notation reads

$$(Q^{L+2k}-1)(\alpha\beta-\gamma\delta Q^{L-2k-2})=0. \tag{4}$$

Here k is an integer such that $|k|\le L/2$. For a given k this constraint can be satisfied by choosing Q to be an appropriate root of unity, or by relating the boundary and bulk parameters such that the second factor in (4) is zero. However, for generic values of the PASEP parameters (4) can also be satisfied by choosing $k=-L/2$. For this choice of k we infer from [18] that for even L there is an isolated level with energy $E_0=0$, the ground state energy of the PASEP. Furthermore, all excited levels are given by

$$E=\alpha+\beta+\gamma+\delta+\sum_{j=1}^{L-1}\frac{\left(Q^2-1\right)^2 z_j}{(Q-z_j)(Qz_j-1)}, \tag{5}$$

where the complex numbers z_j satisfy the Bethe ansatz equations

$$\left[\frac{z_jQ-1}{Q-z_j}\right]^{2L}K(z_j)=\prod_{l\neq j}^{L-1}\frac{z_jQ^2-z_l}{z_j-z_lQ^2}\frac{z_jz_lQ^2-1}{z_jz_l-Q^2}. \tag{6}$$

Here $K(z)=\tilde{K}(z,\alpha,\gamma)\tilde{K}(z,\beta,\delta)$ and

$$\tilde{K}(z,\alpha,\gamma)=\frac{-\alpha z^2+Qz(Q^2-1+\alpha-\gamma)+\gamma Q^2}{\gamma Q^2z^2+Qz(Q^2-1+\alpha-\gamma)-\alpha}. \tag{7}$$

In order to ease notations we have set, without loss of generality, $p=1$ and hence $Q=\sqrt{q}$. We note that in the case of symmetric diffusion $Q=1$ (6) reduce to the Bethe ansatz equations derived in [19] by completely different means. In order to determine the exact value of the spectral gap we have analyzed (5) and (6) in the limit $L\to\infty$. To simplify the analysis, we will focus on the case of total asymmetry $\gamma=\delta=0$, $Q\to 0$ in the remainder of this Letter.

Totally asymmetric exclusion (TASEP): After a rescaling $z\to Qz$ and setting $\gamma=\delta=0$, the $Q\to 0$ limit of equations (5) and (6) reads

$$E=\alpha+\beta+\sum_{l=1}^{L-1}\frac{z_l}{z_l-1}, \tag{8}$$

$$\left(\frac{(z_j-1)^2}{z_j}\right)^L=(z_j+a)\,(z_j+b)\prod_{l\neq j}^{L-1}\left(z_j-z_l^{-1}\right), \tag{9}$$

where $a=(1-\alpha)/\alpha$ and $b=(1-\beta)/\beta$. We define $g(z)=\ln z/(z-1)^2$ and $g_{\rm b}(z)=\ln z/(1-z^2)+\ln(z+a)+\ln(z+b)$, and consider the "counting function" [20],

$$\mathrm{i}Y_L(z)=g(z)+\frac{1}{L}g_{\rm b}(z)+\frac{1}{L}\sum_{l=1}^{L-1}K(z_l,z), \tag{10}$$

where $K(w,z)=-\ln w+\ln(1-wz)$. Equations (9) can now be written as

$$Y_L(z_j)=\frac{2\pi}{L}I_j\quad(j=1,\ldots,L-1), \tag{11}$$

where the I_j are integers. Each set of integers $\{I_j\}$ specifies a particular excited state, and we find numerically that the first excited state is obtained for the choice

$$I_j=-L/2+j\quad\text{for}\quad j=1,\ldots,L-1. \tag{12}$$

The eigenvalue (8) can be written as

$$E=\alpha+\beta+L\lim_{z\to1}\left(\mathrm{i}\,Y_L'(z)-g'(z)-\frac{1}{L}g_{\rm b}'(z)\right). \tag{13}$$

In order to derive an integral equation for $Y_L(z)$ in the limit $L\to\infty$ we write,

$$\frac{1}{L}\sum_{j=1}^{L-1}f(z_j)=\oint_{C_1+C_2}\frac{dz}{4\pi\mathrm{i}}\,f(z)Y_L'(z)\cot\left(\frac{1}{2}LY_L(z)\right), \tag{14}$$

where $C=C_1+C_2$ is a contour enclosing all the roots z_j, C_1 being the "interior" and C_2 the "exterior" part, see Fig. 1. The contours C_1 and C_2 intersect in appropriately chosen points ξ and ξ^*. Using the fact that integration

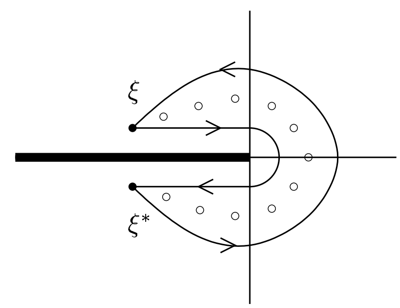

FIG. 1: Sketch of the contour of integration C in (14). The open dots correspond to the roots z_j and ξ is chosen close to z_{L-1} and avoiding poles of $\cot(LY_L(z)/2)$.

from ξ^* to ξ over the contour formed by the roots is equal to half that over C_2-C_1 we find using (14),

$$\begin{aligned}\mathrm{i}\,Y_L(z)\;&=\;g(z)+\frac{1}{L}g_{\rm b}(z)+\frac{1}{2\pi}\int_{\xi^*}^{\xi}K(w,z)Y_L'(w)\mathrm{d}w\\&+\frac{1}{2\pi}\int_{C_1}\frac{K(w,z)Y_L'(w)}{1-\mathrm{e}^{-\mathrm{i}LY_L(w)}}\,\mathrm{d}w\\&+\frac{1}{2\pi}\int_{C_2}\frac{K(w,z)Y_L'(w)}{\mathrm{e}^{\mathrm{i}LY_L(w)}-1}\,\mathrm{d}w,\end{aligned} \tag{15}$$

where we have chosen the branch cut of $K(w,z)$ to lie along the negative real axis. The eigenvalue (13) is obtained by systematically expanding (15) in the system size using standard methods. We note that care has to be taken when there is a stationary point of $Y_L(z)$ close to the contour of integration, in which case an analysis similar to that in [13] has to be carried out.

Let us briefly recall the stationary state phase diagram derived in [8, 9]. There are altogether four phases in the stationary state at $t = \infty$: (1) the low density phase for $\alpha < \beta < 1/2$; (2) the high density phase for $\beta < \alpha < 1/2$; (3) the coexistence line at $\beta = \alpha < 1/2$; (4) the maximal current phase at $\alpha, \beta > 1/2$. We now determine the scaling of the spectral gap in these regimes from the Bethe ansatz equations.

Low and High Density Phases: Let us fix the end points ξ^* and ξ by

$$Y_L(\xi^*) = -\pi + \frac{\pi}{L}, \qquad Y_L(\xi) = \pi - \frac{\pi}{L}. \tag{16}$$

The integral over C_1 in (15) can be calculated by splitting the contour into its upper and lower parts and expanding the integrand around ξ and ξ^* respectively. Expanding in inverse powers of L, i.e.,

$$Y_L(z) = \sum_{n=0} L^{-n} Y_n(z), \qquad \xi = z_{\rm c} + \sum_{n=1} \delta_n L^{-n}, \tag{17}$$

and assuming that $-a < z_{\rm c}$ and $-b < z_{\rm c}$, we find from equation (15) to $\mathcal{O}(L^{-1})$ that,

$$Y_0(z) = -{\rm i} \ln \left[-\frac{z}{z_{\rm c}} \left(\frac{1 - z_{\rm c}}{1 - z} \right)^2 \right], \tag{18}$$

$$Y_1(z) = -{\rm i} \ln \left[-\frac{z}{z_{\rm c}} \frac{1 - z_{\rm c}^2}{1 - z^2} \left[\frac{z_{\rm c} - z_{\rm c}^{-1}}{z - z_{\rm c}^{-1}} \right]^{\nu_1} \frac{z + a}{z_{\rm c} + a} \frac{z + b}{z_{\rm c} + b} \right] - {\rm i} \ln \left(ab(-z_{\rm c})^{\nu_1} \right), \tag{19}$$

where $\nu_1 = -Y_0'(z_{\rm c})\delta_1/\pi$. The values of ν_1 and $z_{\rm c}$ follow from (16) to be $\nu_1 = 2$, $z_{\rm c} = -1/\sqrt{ab}$. Substituting these values into (13) we obtain the gap (20), which is of order $\mathcal{O}(1)$ in the limit $L \to \infty$.

If $-b > -1/\sqrt{ab}$ the point $-b$ lies inside the contour formed by the roots, see Fig 1, giving rise to a different solution for $Y_1(z)$. Comparing again with condition (16) we find in this case that $\nu_1 = 3$ and $z_{\rm c} = -a^{-1/3} = -1/\sqrt{ab_{\rm c}}$, resulting in the spectral gap given in (21), which is independent of β and again of order $\mathcal{O}(1)$ in the limit $L \to \infty$. A similar analysis is made when $-a > -1/\sqrt{ab}$. As the spectral gap is $\mathcal{O}(1)$ in the low and high density phases, the correlation length is finite and these phases are therefore massive.

Coexistence Line: Subleading corrections can be obtained by taking higher order terms into account in (17). After a lengthy calculation we find that the gap vanishes like L^{-2} on the coexistence line $\beta = \alpha$, with a constant of proportionality given by (22).

Maximal Current phase: When $\beta > \beta_{\rm c}$ and $\alpha \to 1/2$, the value of $z_{\rm c}$ where the contour closes approaches $z_{\rm c} = -1$ and a straightforward expansion of the last two terms in (15) breaks down as $Y_L'(\xi^*) \approx Y_0'(-1) = 0$. A further complication is the singularity in $K(w, z)$ at $w = z = z_{\rm c} = -1$. To proceed one expands around $z_{\rm c}$ defined by $Y_L'(z_{\rm c}) = 0$ [13, 21]. This gives rise to an expansion of $Y_L(z)$ in powers of $L^{-1/2}$ and one finds in lowest order that the energy gap vanishes as $L^{-3/2}$. The prefactor can only be determined numerically.

We now summarize our results. We have used Bethe's ansatz to diagonalize the PASEP transition matrix M for arbitrary values of the rates p, q, α, β, γ and δ that characterize the most general PASEP with open boundaries. The resulting Bethe ansatz equations (5), (6) describe the *complete* excitation spectrum of M and are one of our main results. We have carried out a detailed analysis of the Bethe ansatz equations for the simplified case of the TASEP and determined the exact asymptotic behaviour of the spectral gap for large lattice lengths L. This gap determines the long time ($t \gg L$) dynamical behaviour of the TASEP. We emphasize that care has to be taken regarding time scales, and that our results below are not valid at intermediate times $t \approx L$ where the system behaves as for periodic boundary conditions [2].

We found that there are three regions in parameter space where the spectral gap is finite and the stationary state is approached exponentially fast, and one region and a line where the gap vanishes as $L \to \infty$. The resulting dynamical phase diagram is shown in Figure 2. In order to parametrize the phases we define $\beta_{\rm c} = (1 + a^{-1/3})^{-1}$ and $\alpha_{\rm c} = (1 + b^{-1/3})^{-1}$. The values

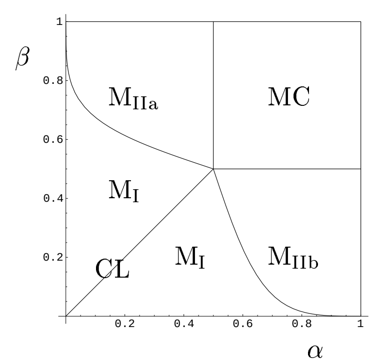

FIG. 2: Dynamic phase diagram of the TASEP. $M_{\rm I}$, $M_{\rm IIa}$ and $M_{\rm IIb}$ are massive phases, CL denotes the critical coexistence line and MC the critical maximal current phase.

of the spectral gap in the various regions of the phase diagram of the TASEP are as follows:

Massive Phase $M_{\rm I}$*:* $\alpha < \alpha_{\rm c}$, $\beta < \beta_{\rm c}$, $\alpha \neq \beta$

$$-E_1 = \alpha + \beta - \frac{2}{1 + \sqrt{ab}} + \mathcal{O}(L^{-2}), \tag{20}$$

The spectral gap does not vanish as $L \to \infty$ and hence implies a finite correlation length and exponential approach to stationarity.

Low Density Phase $M_{\rm IIa}$*:* $\alpha < 1/2$, $\beta > \beta_{\rm c}$

$$-E_1 = \alpha + \beta_{\rm c} - \frac{2}{1 + \sqrt{ab_{\rm c}}} + \mathcal{O}(L^{-2}), \tag{21}$$

Note that in this phase the spectral gap is independent of β. The behaviour in the high-density phase M_{IIb}: $\beta < 1/2$, $\alpha_c < \alpha$ is obtained by the exchange $\alpha \leftrightarrow \beta$.

Coexistence Line (CL): $\beta = \alpha < 1/2$.

$$-E_1 = \frac{\pi^2\alpha(1-\alpha)}{1-2\alpha}L^{-2} + \mathcal{O}(L^{-3}). \qquad (22)$$

We thus find a dynamic exponent $z = 2$ corresponding to diffusive behaviour.

Maximal Current Phase (MC): $\alpha, \beta > 1/2$.

$$-E_1 \approx 3.56L^{-3/2} + \mathcal{O}(L^{-2}). \qquad (23)$$

In this phase, which coincides with the stationary maximum current phase, we find a KPZ [22] dynamic exponent $z = 3/2$. The gap is smaller than that of the periodic case where it is found that $-E_1 = 6.509\ldots L^{-3/2}$ [13, 23]. We note that the subdivision of the massive high and low density phases is different from the one suggested on the basis of stationary state properties in [9].

Discussion: It is known [24] that by varying the bulk hopping rates one can induce a crossover between a diffusive Edwards-Wilkinson (EW) scaling regime [25] with dynamic exponent $z = 2$ and a KPZ regime [22] with $z = 3/2$. In this letter we have shown using exact methods that a crossover between phases with $z = 2$ and $z = 3/2$ occurs in the case where the bulk transition rates are kept constant, but the boundary injection/extraction rates are varied. As shown in [15] the diffusive relaxation ($z = 2$) is of a different nature than in the EW regime and is in fact due to the unbiased random walk behaviour of a shock (domain wall between a low and high density region). Our results (20) and (22) for the massive phase M_I and the coexistence line agree with the relaxation time calculated in the framework of a domain wall theory (DWT) model in [15]. This is in contrast to the massive phases M_{II}, where the exact result (21) differs from the DWT prediction. An interesting open question is whether it is possible to understand (21) in a generalized DWT framework.

The Bethe ansatz equations (5), (6) allow for the exact determination of further spectral gaps. We find that the eigenvalue of the transition matrix with the next largest real part is complex, which leads to interesting oscillatory behaviour at large times. The dynamical phase diagram for the general PASEP is expected to be significantly richer, and its analysis is under way.

The condition (4) is a reflection of the non-semisimplicity of an underlying Temperley-Lieb algebra with two additional boundary generators [26]. Remarkably the PASEP satisfies this constraint for arbitrary values of its parameters. Generically, non-semisimplicity implies certain symmetries in the spectrum, and the physical consequences of these are currently under investigation.

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