Large Deviation Function for the Current in the Open Asymmetric Simple Exclusion Process

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Current large deviation function for the open asymmetric simple exclusion process

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We consider the one dimensional asymmetric exclusion process with particle injection and extraction at two boundaries. The model is known to exhibit four distinct phases in its stationary state. We analyze the current statistics at the first site in the low and high density phases. In the limit of infinite system size, we conjecture an exact expression for the current large deviation function.

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Introduction. One of the main open problems in classical statistical physics is the formulation and derivation of simple laws that determine macroscopic quantities in strongly interacting systems far from equilibrium. A broad class of nonequilibrium systems can be characterized by the presence of a macroscopic current. An important diagnostic tool of non-equilibrium behaviour is then provided by the probability distribution of current fluctuations. The latter is suitably represented in terms of its moments, which are encoded in the current large deviation function (LDF). LDFs play an important role in the application of fluctuation theorems [1–3]. Microscopic models of interacting particles provide a useful framework for studying non-equilibrium properties in current-carrying classical systems and have become a major subject of research over the past two decades. One of their main uses is that their large deviation properties can be derived microscopically, which furnishes rigorous tests of underlying assumptions in phenomenological approaches.
The asymmetric simple exclusion process (ASEP), describing the asymmetric diffusion of hard-core particles along a one-dimensional chain, is one of the best studied paradigms of non-equilibrium Statistical Mechanics [4]. The ASEP is of general interest due to its close relation to growth phenomena [5], as observed in recent experiments on electroconvection [6]. It is also used as a model of molecular diffusion in zeolites [7], of biopolymers [8] and sequence alignment [9], traffic flow [10] and quantum dot chains [11]. The exact probability distribution for current fluctuations for the ASEP on a ring has been known for some time [12]. In the open boundary ASEP phenomenological [13], approximate [11] and numerical [14] treatments have been developed, but the determination of the current LDF from first principles has been one of the outstanding problems in the field. Despite considerable effort, the LDF is only known in the limiting cases of symmetric exclusion [15] and weak asymmetry [16]. For the infinite system the time dependence was obtained for total asymmetry in [17].

Definition of the ASEP. 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 ($i = 2, \dots, L-1$) 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 by allowing particles to enter (leave) with rates α (γ) at site $i = 1$ and with rates δ (β) at site $i = L$ respectively, see Figure 1.

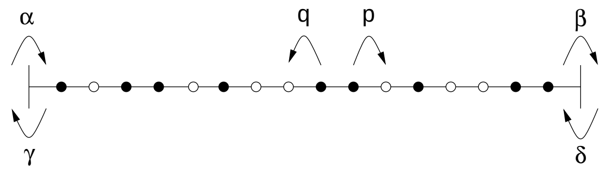

FIG. 1: Dynamical rules of the ASEP.

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 $P_t(\tau_1, \dots, \tau_L)$. The time evolution of P_t occurs according to the aforementioned rules and is subject to the master equation

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

Here $M = m_1 + m_L + m_{\text{bulk}}$ is the ASEP transition matrix whose eigenvalues have non-positive real parts. The late time behaviour of the ASEP is dominated by the eigenstates of M with the largest real parts of the corresponding eigenvalues [18]. The boundary contributions m_1 and m_L describe injection (extraction) of particles at sites 1 and L. In the following we use a more convenient parametrization in terms of the quantities $a = \kappa^+_{\alpha,\gamma}$, $b = \kappa^+_{\beta,\delta}$, $c = \kappa^-_{\alpha,\gamma}$, $d = \kappa^-_{\beta,\delta}$, where

$$\kappa^{\pm}_{\alpha,\gamma} = \frac{p-q-\alpha+\gamma \pm \left[(p-q-\alpha+\gamma)^2 + 4\alpha\gamma\right]^{\frac{1}{2}}}{2\alpha}. \tag{2}$$

Stationary state properties of the ASEP. At late times the ASEP approaches a stationary state. Physical properties then depend sensitively on the boundary conditions [19]. For $q < p$ one finds four different phases

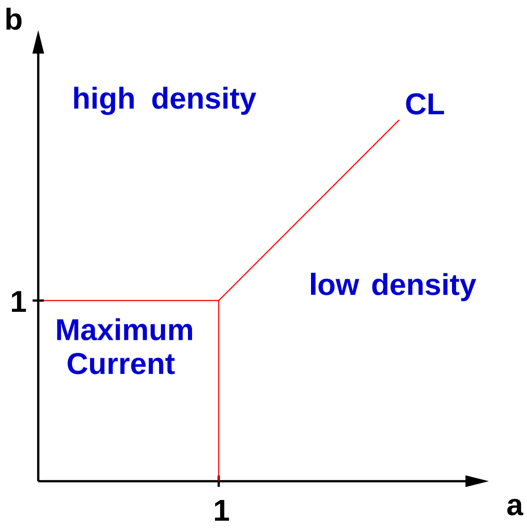

FIG. 2: Stationary state phase diagram for the ASEP. On the coexistence line (CL) a first order phase transition occurs.

as a function of the boundary rates as is shown in Fig.2.

Current Fluctuations. We are interested in the probability distribution of the total time-integrated current $Q_1(t)$, i.e. the net number of particle jumps between the left boundary reservoir and site 1 in the time interval $[0,t]$. The moments of the distribution are encoded in the generating function $\langle \mathrm{e}^{\lambda Q_1(t)}\rangle$, where the brackets denote an average over all histories. In this Letter we report an explicit expression for the quantity

$$E(\lambda) = \lim_{L\to\infty}\lim_{t\to\infty}\frac{1}{t}\log\langle \mathrm{e}^{\lambda Q_1(t)}\rangle. \qquad (3)$$

This characterizes the asymptotic current distribution which, for an ergodic system, is not expected to depend on the choice of initial particle configuration.

As observed in [20], eqn (3) implies a large deviation property for the probability distribution $P(j_1,t)$ of the average current $j_1 = Q_1(t)/t$ at the first site. The long-time limiting behaviour is given by $P(j_1,t) \sim \mathrm{e}^{-t\widehat{E}(j_1)}$ where $\widehat{E}(j_1) = \max_\lambda\{\lambda j_1 - E(\lambda)\}$ is the Legendre transform of $E(\lambda)$. As a tool to compute the current LDF we introduce a fugacity e^λ conjugate to the current on the first site. The boundary term m_1 then becomes

$$m_1 = \begin{pmatrix} -\alpha & \gamma \mathrm{e}^{-\lambda} \\ \alpha \mathrm{e}^{\lambda} & -\gamma \end{pmatrix} \otimes \mathbb{I}_{L-1}, \qquad (4)$$

and $E(\lambda)$ is equal to the largest eigenvalue of the generalized "transition matrix" $M(\lambda)$. The spectrum of $M(\lambda)$ obeys a Gallavotti-Cohen symmetry [1, 2, 18, 20]: the eigenvalues of $M(\lambda')$ and $M(\lambda)$ are equal when λ' and λ are related by $\mathrm{e}^{\lambda'} = abcdq^{L-1}\mathrm{e}^{-\lambda}$.

Summary of Results. Our main result is that the generating function (3) for current fluctuations at site 1 in the low and high density phase and for small λ and $L\to\infty$ is of the form

$$E(\lambda) = (p-q)\frac{a(\mathrm{e}^\lambda - 1)}{(1+a)(\mathrm{e}^\lambda + a)}. \qquad (5)$$

In the high density phase we obtain the same expression with a replaced by b. Note that the requirements that λ is small and $L\to\infty$ explicitly break the Gallavotti-Cohen symmetry, as this is a duality between small and large negative λ. We may use (5) to derive explicit expressions for the first few cumulants of the local current in terms of the average bulk density $\rho = 1/(1+a)$,

$$\begin{aligned}
&\lim_{t\to\infty}\frac{\langle Q_1\rangle}{t} = (p-q)\rho(1-\rho),\\
&\lim_{t\to\infty}\frac{\langle Q_1^2\rangle - \langle Q_1\rangle^2}{t} = (p-q)\rho(1-\rho)(1-2\rho),\\
&\lim_{t\to\infty}\frac{\langle Q_1^3\rangle - 3\langle Q_1^2\rangle\langle Q_1\rangle + \langle Q_1\rangle^3}{t} =\\
&\qquad (p-q)\Big[\rho - 7\rho^2 + 12\rho^3 - 6\rho^4\Big]. \qquad (6)
\end{aligned}$$

The first result reproduces, as expected, the bulk current [19], while the second moment agrees with the diffusion constant in the limit $q\to 0$ of completely asymmetric diffusion [21].

Derivation. In the following we set $p=1$ without loss of generality. Based on earlier work on the quantum XXZ spin chain [22], the generalized ASEP transition matrix was shown to be diagonalizable using the Bethe ansatz in the case where the parameters satisfy [18, 23]

$$\left(q^{L/2+k} - \mathrm{e}^\lambda\right)\left(\alpha\beta \mathrm{e}^\lambda - q^{L/2-k-1}\gamma\delta\right) = 0. \qquad (7)$$

Here k is an arbitrary integer in the interval $|k| \le L/2$. By considering small finite systems we find that the largest eigenvalue $E(\lambda)$ is described by one of the sets of Bethe equations given in [18], which can be cast in the form

$$\begin{aligned}
E &= \sum_{l=1}^{L/2+k}\frac{(1-q)^2 z_l}{(1-z_l)(1-qz_l)} \equiv \sum_{l=1}^{n}\varepsilon(z_l), && (8)\\
Y_L(z_j) &= \frac{2\pi}{L}I_j, \quad j = 1\ldots,\frac{L}{2}+k, && (9)
\end{aligned}$$

where $n = L/2+k$, and $Y_L(z)$ is given by

$$\begin{aligned}
\mathrm{i}\,Y_L(z) &= g(z) + \frac{1}{L}g_b(z) - \left(1 - \frac{n-1}{L}\right)\ln(-qz)\\
&\quad + \frac{1}{L}\sum_{l=1}^{n}K(z_l,z). \qquad (10)
\end{aligned}$$

Here the functions g, g_b and K are given by

$$g(z) = \ln\left[z\frac{(1-qz)^2}{(1-z)^2}\right], \qquad (11)$$

$$g_b(z) = \ln\left[-\frac{1+az}{a+qz}\frac{1+cz}{c+qz}\right] + \ln\left[-\frac{1+bz}{b+qz}\frac{1+dz}{d+qz}\right] + \ln\left[\frac{1}{z}\frac{1-q^2z^2}{1-z^2}\right]. \qquad (12)$$

$$K(w,z) = -\ln(w) - \ln\left(\frac{1-qz/w}{1-qw/z}\frac{1-q^2wz}{1-wz}\right). \qquad (13)$$

We note that these equations are different from those describing the low lying excitations of the ASEP [18].

The constraint (7) can be satisfied for arbitrary $\alpha, \beta, \gamma, \delta$, q and k by fixing the parameter λ characterizing the generating function to a value among the sequences (S1) $\lambda_n^{(1)} = n\ln(q)$ or (S2) $\lambda_n^{(2)} = \ln\left(\gamma\delta q^{n-1}/\alpha\beta\right)$, where n is an integer with $0 \le n \le L$. In order to infer $E(\lambda)$ we employ the following strategy: we set $\lambda = \lambda_n^{(j)}$ and then determine the ground state energies $E(\lambda_n^{(j)})$ of the corresponding generalized transition matrices. From the sequences of values obtained in this manner we then conjecture a general expression for $E(\lambda)$.

Ground State Energy for sequence (S1). Here, the ground state in the low density phase corresponds to a solution of the Bethe ansatz equations with only n roots ($n = 1, 2, \ldots$)

$$z_j = -\frac{q^{j-1}}{a} + \mathcal{O}\left(e^{-\mu_j L}\right), \quad j = 1, \ldots, n, \qquad (14)$$

where for large L the μ_j approach constant values. We have checked (14) against exact diagonalization of small chains ($L \le 14$) for many values of the boundary rates and $n \le 5$. We conjecture that it is correct in general for sufficiently small n, i.e. n such that $q^{2n} > abcdq^{L-1} = \gamma\delta q^{L-1}/\alpha\beta$. The solution (14) is of the form of a maximal *boundary bound state*: one root lies exponentially close to a pole of the boundary phase shift $e^{g_b(z)}$, while pairs of the others lie on poles of the two-particle phase shift $e^{K(z_k, z_l)}$. The ground state energy (8) becomes

$$E = \sum_{j=0}^{n-1} \epsilon\left(-\frac{q^{j-1}}{a}\right) = (1-q)\left(\frac{a}{a+1} - \frac{a}{a+q^n}\right). \qquad (15)$$

Restoring λ and p we obtain the result (5).

Ground State Energy for sequence (S2). Here the analysis is considerably more involved. The ground state in the low density phase is again given by (8), (9), but now with $k = L/2 - n$. To keep $\lambda_n^{(2)}$ small for $L \gg 1$ we require $n \ll L$, which corresponds to the number of Bethe roots being $\mathcal{O}(L)$. In the following we present details for the case $n = 1$, other values can be treated analogously. For $n = 1$ there are $L - 1$ roots. The ground state is obtained by choosing

$$I_j = -L/2 + j, \qquad j = 1, \ldots, L-1. \qquad (16)$$

The corresponding roots lie on a contour that closes as $L \to \infty$ on a point z_c on the negative real axis, see e.g. the plot on the left hand side of Figure 3.

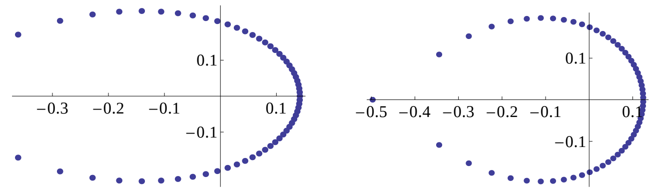

FIG. 3: Distribution of reciprocal roots $1/z_j$ for $L = 60$. Left: $a = 3.45$, $b = 1.5$, $c = -0.55$, $d = -0.6$ and $q = 0.8$. Right: $a = 1.7$, $b = 1.6$, $c = -0.55$, $d = -0.6$ and $q = 0.9$. Both contours close on the negative real axis as L increases.

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Following [18] we obtain an integro-differential equation for the root density $Y_L(z)$ in the limit $L \to \infty$, valid in the low and high density phases. Dropping subleading contributions in L^{-1} we have

$$\mathrm{i}\, Y_L(z) = g(z) + \frac{1}{L}g_{\mathrm{b}}(z) + \frac{1}{2\pi}\int_{\xi^-}^{\xi^+} K(w,z)Y_L'(w)\delta w. \qquad (17)$$

The integral from ξ^- to ξ^+ is along the contour formed by the roots, and the end points are fixed by $Y_L(\xi^\pm) = \pm(\pi - \pi/L)$. Equation (17) may be solved by expanding in powers of L^{-1}, i.e. $Y_L(z) = y_0(z) + y_1(z)/L + \ldots$, $\xi = z_c + (\delta + \mathrm{i}\,\eta)/L + \ldots$, which upon substitution into (17) yield integro-differential equations for the functions y_0 and y_1. Once these have been determined the corresponding eigenvalue $E(\lambda_n^{(2)})$ is obtained from

$$E = -\frac{L}{2\pi}\oint_{z_c} \varepsilon(z)Y_L'(z)\delta z - \frac{\mathrm{i}}{\pi}y_0'(z_c)\,\eta\,\varepsilon(z_c) + \ldots, \qquad (18)$$

where we have dropped terms of $\mathcal{O}(L^{-1})$. Here, the integral is over the closed contour on which the roots lie.

Assumption I: $\lambda > 0$, $-1/a$ inside the contour. This regime corresponds to the case where $e^\lambda = abcd > 1$, and is defined by assuming that $-1/a$ lies inside the contour of integration and all other poles of g_{b} lie outside. The zeroth order term in the expansion of the counting function can be found as in [18], and is given by

$$y_0(z) = -\mathrm{i}\ln\left[-\frac{z}{z_c}\left(\frac{1-z_c}{1-z}\right)^2\right]. \qquad (19)$$

Under the above assumption, the driving term of the subleading integro-differential equation can be shown to have branch points at $-1/a$ and at qz_c. The branch point at $-1/a$ results in branch points in $y_1(z)$ at the points $-q^m/a$, $m = 0, 1, 2\ldots$, and likewise for the branch point at qz_c. As in [18], this suggests a functional form for $y_1(z)$ which may then be obtained explicitly.

Finally, employing the boundary conditions for $\xi^\pm$, it is possible to show that in this regime $\delta = 0$, $\eta\, y_0'(z_c) = \mathrm{i}\pi$ and that the contour closes at $z_c = -bcd$, which agrees well with numerical solutions of (9) up to $L = 200$. The energy can be computed from (18) and is given by

$$E = (1-q)\left(\frac{a}{a+1} - \frac{1}{1-z_{\rm c}}\right), \tag{20}$$

which with $z_{\rm c} = -bcd$ is fully consistent with (5), and coincides with it when we restore p and λ using $e^{\lambda} = abcd$.

Assumption II: $\lambda < 0$, $g_{\rm b}$ analytic inside the contour. A numerical analysis of the case $e^{\lambda} = abcd < 1$ indicates that the roots again lie on a contour, except for isolated roots on the negative real axis. Fig. 3 gives an example with one such isolated root $z_1 \approx -1/a$. Assuming that the boundary term $g_{\rm b}$ does not have poles inside the contour, the leading order integro-differential equations may again be obtained explicitly. While the details are slightly different from above, the final result is again (20) with $z_{\rm c} = -bcd$, confirming also in this case (5).

Conclusions. We have presented a conjecture for the exact current LDF in the high and low density phases of the ASEP with open boundaries in the limit of infinite system size. After our manuscript appeared on arXiv, (5) has been confirmed by two indepedent approaches: Bodineau and Derrida informed us that they succeeded in obtaining our result in the framework of their macroscopic approach [16] and in a recent preprint [26] the current LDF for the totally asymmetric exclusion process on a finite lattice was calculated using an extension of the matrix product method. While the density LDF for the open ASEP has been known for some time [24], the exact determination of its current LDF has been an important outstanding problem. Both quantities are assumed to fully describe the experimentally accessible macroscopic behaviour of the ASEP [6]. So far we have not been able to access the coexistence line and the maximum current phase, where it is necessary to scale the parameter λ with system size [12]. In the maximum current phase we can analyze only the limit $L \to \infty$ for fixed λ, where $E(\lambda) = (p-q)\tanh(\lambda/4)$. It would be interesting to see whether progress can be made for weak asymmetry, c.f. [25]. Finally we note that we have obtained preliminary results on finite-size corrections to (5).

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