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Bethe ansatz solution for a defect particle in the asymmetric exclusion process

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Abstract. The asymmetric exclusion process on a ring in one dimension is considered with a single defect particle. The steady state has previously been solved by a matrix product method. Here we use the Bethe ansatz to solve exactly for the long time limit behaviour of the generating function of the distance travelled by the defect particle. This allows us to recover steady state properties known from the matrix approach such as the velocity, and obtain new results such as the diffusion constant of the defect particle. In the case where the defect particle is a second-class particle we determine the large deviation function and show that in a certain range the distribution of the distance travelled about the mean is Gaussian. Moreover, the variance (diffusion constant) grows as $L^{1/2}$ where L is the system size. This behaviour can be related to the superdiffusive spreading of excess mass fluctuations on an infinite system. In the case where the defect particle produces a shock, our expressions for the velocity and the diffusion constant coincide with those calculated previously for an infinite system by Ferrari and Fontes.

1. Introduction and model definition

The asymmetric simple exclusion process (ASEP) [1] is a simple example of a driven lattice gas [2] and as such is a system far from thermal equilibrium. The model comprises particles hopping in a preferred direction along a one-dimensional lattice with hard core exclusion imposed. The model's broad interest lies in its connections to growth processes, the problem of directed polymers in a random medium and Burgers equation [3, 4]. It is also a natural starting point for many traffic flow models [5].

Multi-species variants of the ASEP have been considered [6–10]. In particular the idea of a second-class particle has proven useful [6]. The second-class particle hops forward as usual when the neighbouring site is empty but is overtaken by the other particles. Therefore, it moves forward in an environment of low density of particles and backwards in a high-density environment. In this way a second-class particle can be used to locate shocks which are sudden changes in density over a microscopic region [11–14]. A generalization of the second-class particle idea to that of a defect particle [15, 16] has been shown to exhibit phase transitions and, in particular, phase coexistence. Interpreted in the context of traffic problems, the phase transition corresponds to the appearance of a traffic jam whereas coexistence between phases of different densities corresponds to the coexistence between a freely flowing and a jammed region in traffic. The model has also been interpreted in the context of a two-way road [17].

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Analytical results for the ASEP, such as the steady state of systems with open boundaries [18, 19], the diffusion constant [20], and the steady state for the second-class particle problem [6, 15, 16] have been obtained via a matrix product technique [18, 21]. Recently it was shown that a Bethe ansatz aprroach to the ASEP, used previously to calculate the gap and dynamic exponent [22–24], could be extended to obtain all moments and the large deviation function of the time integrated current [25–27]. Here we show that the Bethe ansatz can also be used in the case of the defect particle and this allows us to generalize previous [15, 16, 28] results obtained by the matrix approach.

Let us now define the model we consider [15, 16]. The model comprises a single defect particle (indicated by 2) and $M-1$ first-class (i.e. normal) particles (indicated by 1) on a ring of size L sites. The hopping rates of the particles are as follows

$$\begin{array}{lll} 10 \to 01 & \text{with rate} & 1 \\ 20 \to 02 & \text{with rate} & \alpha \\ 12 \to 21 & \text{with rate} & \beta . \end{array} \tag{1}$$

By this it is implied, for example, that in an infinitessimal time interval, dt, a first-class particle hops to the neighbouring site to the right with probability dt if that neighbouring site is empty. We restrict ourselves to $\alpha, \beta > 0$.

2. Main results

Before discussing the technical details of the Bethe ansatz solution we summarize in this section our main results. Let us denote by y_t the distance travelled (total number of hops forward minus total number of hops backward) by the defect particle. In the steady state, y_t is a random variable. Its first and second moments give the velocity v and the diffusion constant Δ of the defect particle:

$$v = \lim_{t\to\infty} \frac{\langle y_t \rangle}{t} \tag{2}$$

$$\Delta = \lim_{t\to\infty} \frac{\langle y_t^2 \rangle - \langle y_t \rangle^2}{t}. \tag{3}$$

All cumulants of y_t can be computed from the knowledge of the generating function $\langle e^{\gamma y_t} \rangle$ via

$$\langle y_t^n \rangle_c = \left. \frac{d^n \ \ln[\langle e^{\gamma y_t} \rangle]}{d\gamma^n} \right|_{\gamma=0}. \tag{4}$$

Here, by employing a Bethe ansatz technique we calculate exactly the large t behaviour of this generating function namely

$$\lambda(\gamma) = \lim_{t\to\infty} \frac{\ln[\langle e^{\gamma y_t} \rangle]}{t} \tag{5}$$

for arbitrary L and M. Exact expressions of v and Δ follow easily from the knowledge of $\lambda(\gamma)$:

$$v = \left. \frac{d}{d\gamma} \lambda(\gamma) \right|_{\gamma=0} \qquad \Delta = \left. \frac{d^2}{d\gamma^2} \lambda(\gamma) \right|_{\gamma=0}. \tag{6}$$

In the thermodynamic limit (L, M large) with fixed density ρ where

$$\rho = M/L \tag{7}$$

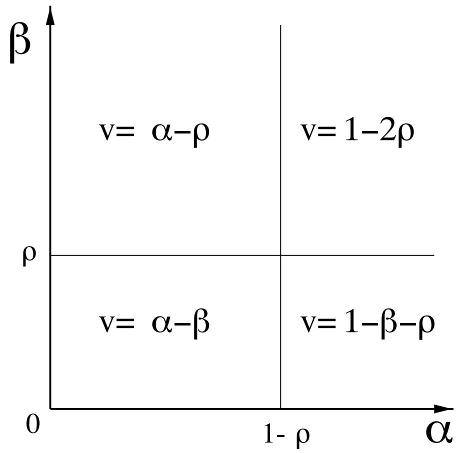

Figure 1. Phase diagram for the model. The velocities in the various phases are indicated.

our exact expressions for $\lambda(\gamma)$ allow us to show that the velocity v and diffusion constant Δ of the defect particle have the following asymptotic forms in different regions of the parameter space of α, β, ρ:

$$\text{For}\quad \beta > \rho \quad \text{and} \quad \alpha > 1-\rho \qquad v \to 1-2\rho \quad \text{and} \quad \frac{\Delta}{L^{1/2}} \to \frac{(\pi\rho(1-\rho))^{1/2}}{4} \tag{8}$$

$$\text{For}\quad \beta < \rho \quad \text{and} \quad \alpha > 1-\rho \qquad v \to 1-\beta-\rho \quad \text{and} \quad \Delta \to \frac{\beta(1-\beta)}{\rho-\beta} \tag{9}$$

$$\text{For}\quad \beta > \rho \quad \text{and} \quad \alpha < 1-\rho \qquad v \to \alpha-\rho \quad \text{and} \quad \Delta \to \frac{\alpha(1-\alpha)}{1-\rho-\alpha} \tag{10}$$

$$\text{For}\quad \beta < \rho \quad \text{and} \quad \alpha < 1-\rho \qquad v \to \alpha-\beta \quad \text{and} \quad \Delta \to \frac{\beta(1-\beta)+\alpha(1-\alpha)}{1-\alpha-\beta}. \tag{11}$$

These results lead to a phase diagram (see figure 1) which has the same expressions for the velocity and is the same upto labelling of phases as that given in [16]. For $\beta > \rho$ and $\alpha > 1-\rho$ it is known [6, 16] that the density profile, as seen from the defect particle, has a power law decay towards its asymptotic value. In the two phases $\beta > \rho$ and $\alpha < 1-\rho$ or $\beta < \rho$ and $\alpha > 1-\rho$ the density profile decays exponentially towards the asymptotic values. In the final phase there is coexistence between a region of low density, β, in front of the defect particle and high density, $1-\alpha$, behind the defect particle. Therefore, there is a shock separating the two regions at a distance xL in front of the defect particle where x is given by $\rho = \beta x + (1-\alpha)x$ [15, 16]. The novelty of this work is that, as we can calculate $\lambda(\gamma)$, all the higher cumulants of the distance travelled (including the diffusion constant) can be calculated exactly for the different phases.

One should notice from (8) that in the whole phase $\beta > \rho$ and $1-\alpha < \rho$ (which includes the case of a second-class particle $\beta = \alpha = 1$) the diffusion constant of the defect particle increases with L. This is in contrast with the diffusion constant of the first-class particles [20, 25] which (in the absence of a defect) decreases as $L^{-1/2}$. This difference between first- and second-class particles is not a surprise since, for an infinite system, one expects the fluctuations of position to be superdiffusive for second-class particles and subdiffusive for first-class particles [29, 30].

Furthermore, in the whole phase $1-\alpha < \rho < \beta$ we will show that $\lambda(\gamma)$ defined by (5) is given in the large L limit by

$$\lambda(\gamma) - \gamma(1-2\rho) \simeq \frac{2\gamma}{L}\left[2-\rho\left(1+\frac{1-\beta}{\rho-\beta}+\frac{\alpha}{\alpha-1+\rho}\right)\right] + \gamma^2 L^{1/2}\frac{\sqrt{\pi\rho(1-\rho)}}{8} \tag{12}$$

on the scale where $\gamma \sim \mathrm{O}(L^{-3/2})$.

The fact that in a certain range γ, the expression of $\lambda(\gamma)$ is quadratic implies that the distribution of the variable $y_t/t - (1-2\rho)$ is Gaussian over a certain range. It is easy to check that the range which corresponds to $\gamma \sim \mathrm{O}(L^{-3/2})$ is $y_t/t - (1-2\rho) \sim \mathrm{O}(1/L)$, so that over that range, the distribution of this difference should be Gaussian.

In the following sections we give the derivation of (8)–(12).

3. Generating function for fluctuations in distance travelled

To calculate $\lambda(\gamma)$, we follow and extend the technique of [25, 26]. First, consider $P_\mathrm{t}(\mathcal{C}, y)$ which is the probability of the system being in configuration $\mathcal{C}$ and of the defect particle having been displaced a distance y (negative if the particle has been displaced backwards). The master equation is

$$\frac{\mathrm{d}P_\mathrm{t}\,(\mathcal{C}, y)}{\mathrm{d}t} = \sum_{\mathcal{C}'}[\mathcal{M}_0(\mathcal{C},\mathcal{C}')P_\mathrm{t}(\mathcal{C}', y) + \mathcal{M}_1(\mathcal{C},\mathcal{C}')P_\mathrm{t}(\mathcal{C}', y-1) + \mathcal{M}_{-1}(\mathcal{C},\mathcal{C}')P_\mathrm{t}(\mathcal{C}', y+1)] \tag{13}$$

where $\mathcal{M}_0(\mathcal{C},\mathcal{C}'), \mathcal{M}_1(\mathcal{C},\mathcal{C}'), \mathcal{M}_{-1}(\mathcal{C},\mathcal{C}')$ are rates for transitions from $\mathcal{C}'$ to $\mathcal{C}$ that do not move the defect particle, move the defect particle forward, move the defect particle backward, respectively. The total rate out of configuration $\mathcal{C}$ is given by $-\mathcal{M}_0(\mathcal{C},\mathcal{C}) = \sum_{\mathcal{C}'\neq\mathcal{C}}[\mathcal{M}_1(\mathcal{C}',\mathcal{C}) + \mathcal{M}_0(\mathcal{C}',\mathcal{C}) + \mathcal{M}_{-1}(\mathcal{C}',\mathcal{C})]$. The generating function

$$F_\mathrm{t}(\mathcal{C}) = \sum_{y=-\infty}^{+\infty} \exp(\gamma y) P_\mathrm{t}(\mathcal{C}, y) \tag{14}$$

obeys

$$\frac{\mathrm{d}F_\mathrm{t}\,(\mathcal{C})}{\mathrm{d}t} = \sum_{\mathcal{C}'}[\mathcal{M}_0(\mathcal{C},\mathcal{C}')F_\mathrm{t}(\mathcal{C}') + \mathrm{e}^{\gamma}\mathcal{M}_1(\mathcal{C},\mathcal{C}')F_\mathrm{t}(\mathcal{C}') + \mathrm{e}^{-\gamma}\mathcal{M}_{-1}(\mathcal{C},\mathcal{C}')F_\mathrm{t}(\mathcal{C}')]. \tag{15}$$

Now

$$\langle \mathrm{e}^{\gamma y_t}\rangle = \sum_{\mathcal{C}} F_t(\mathcal{C}) \tag{16}$$

so we expect as in (5)

$$\langle \mathrm{e}^{\gamma y_t}\rangle \sim \mathrm{e}^{\lambda(\gamma)t} \tag{17}$$

where $\lambda(\gamma)$ is the largest eigenvalue of the matrix $\mathcal{M}(\gamma) = \mathcal{M}_0 + \mathrm{e}^{\gamma}\mathcal{M}_1 + \mathrm{e}^{-\gamma}\mathcal{M}_{-1}$. For $\gamma = 0$ we know that $\lambda(\gamma) = 0$ because $\mathcal{M}(0)$ is a stochastic matrix. Now as in [25,26], by the Perron–Frobenius theorem we know that the largest eigenvalue of $\mathcal{M}(\gamma)$ is non-degenerate therefore as γ increases from zero there can be no crossing of the largest eigenvalue. Thus $\lambda(\gamma)$ is the eigenvalue that tends to zero as γ tends to zero.

One should note in the present problem that for $\gamma = 0$ the eigenvector with eigenvalue zero (the steady state) is non-trivial and has previously been constructed by using a matrix product [6, 16]. In the following sections we show how the Bethe ansatz can recover some properties of this steady state in the limit $\gamma \to 0$.

4. Bethe ansatz

Let a configuration of the particles on the ring be specified by the coordinates $\{x_1, x_2, \ldots, x_M\}$ where x_1 is the position of the defect particle and $x_2 < x_3 \cdots < x_M$ are the positions of the normal particles. By convention, one can always choose $\{x_1 \ldots x_M\}$ such that $1 \leqslant x_1 \leqslant L$ and $x_1 < x_2 < \cdots < x_M < x_1 + L$. With the dynamics (1) the equation for an eigenfunction $\psi(x_1, \ldots x_M)$ of $\mathcal{M}(\gamma)$ with eigenvalue $\lambda(\gamma)$ takes the form: for $x_i < x_{i+1} - 1$ and $x_M < L + x_1 - 1$ (i.e. when all particles are more than one lattice spacing apart):

$$\lambda\psi(x_1, \ldots x_M) = -(M - 1 + \alpha)\psi(x_1, \ldots x_M) + \mathrm{e}^{\gamma}\alpha\psi(x_1 - 1, \ldots x_M) + \sum_{i=2}^{M} \psi(x_1, \ldots, x_i - 1, \ldots x_M). \tag{18}$$

When $x_i = x_{i+1} - 1$ or $x_M = x_1 + L - 1$ (i.e. for configurations where two consecutive sites are occupied), equation (18) is in principle modified. Insisting that it remains valid even in these particular cases, requires that the function $\psi(x_1, \ldots x_M)$ take values in unphysical regions ($x_{i+1} = x_i$ or $x_M = x_1 + L$) which satisfy the following conditions arising from the interaction of particles:

$$(1 - \beta)\psi(x_1, \ldots x_1 + L - 1) - \mathrm{e}^{\gamma}\alpha\psi(x_1 - 1, \ldots x_1 + L - 1) = 0 \tag{19}$$

$$\psi(\ldots, x_i, x_i + 1, \ldots) - \psi(\ldots, x_i, x_i, \ldots) = 0 \qquad \text{for} \quad 1 < i < M \tag{20}$$

$$\alpha\psi(x_1, x_1 + 1 \ldots) - \psi(x_1, x_1 \ldots) + \mathrm{e}^{-\gamma}\beta\psi(x_1 + 1, x_3, \ldots, x_1 + L) = 0. \tag{21}$$

The Bethe ansatz consists of writing the eigenfunction $\psi(x_1, \ldots x_M)$ as

$$\psi(x_1, \ldots x_M) = \mathrm{e}^{\gamma x_1}\alpha^{x_1} \sum_{Q} \mathcal{A}_{Q(1)\ldots Q(M)} (z_{Q(1)})^{x_1} \ldots (z_{Q(M)})^{x_M} \tag{22}$$

where the sum is over all permutations Q of $1 \ldots M$. The amplitudes $\mathcal{A}_{Q(1)\cdots Q(M)}$ and the wave numbers $z_1 \ldots z_M$ are *a priori* arbitrary complex numbers. This ansatz inserted into (18) gives for the eigenvalue

$$\lambda(\gamma) = -(M - 1 + \alpha) + \sum_{k=1}^{M} \frac{1}{z_k} \tag{23}$$

for any choice of the amplitudes $\mathcal{A}_{Q(1)\ldots Q(M)}$ and of the wavenumbers $z_1 \ldots z_M$. For (22) to fulfil conditions (19)–(21), the amplitudes and the wavenumbers have to satisfy:

$$\mathcal{A}_{j\ldots i} = (-)\frac{z_j^L}{z_i^L}\frac{[(1-\beta)z_i - 1]}{[(1-\beta)z_j - 1]}\mathcal{A}_{i\ldots j} \tag{24}$$

$$\mathcal{A}_{\ldots ji\ldots} = (-)\frac{z_j - 1}{z_i - 1}\,\mathcal{A}_{\ldots ij\ldots} \tag{25}$$

$$\mathcal{A}_{ji\ldots} = (-)\frac{1}{(\alpha z_i - 1)}[(\alpha z_j - 1)\mathcal{A}_{ij\ldots} + \alpha\beta z_i z_j^L \mathcal{A}_{i\ldots j} + \alpha\beta z_j z_i^L \mathcal{A}_{j\ldots i}]. \tag{26}$$

Using (24) and (25) allows (26) to be written as

$$\mathcal{A}_{ji\ldots} = (-)\frac{(\alpha z_j - 1)}{(\alpha z_i - 1)}\left[1 + \alpha\beta\frac{z_j^L}{(\alpha z_j - 1)(bz_j - 1)(z_j - 1)^{M-1}}\frac{z_j - z_i}{z_i - 1}\prod_{k=1}^{M}(1 - z_k)\right]\mathcal{A}_{ij\ldots} \tag{27}$$

where

$$b = (1 - \beta). \tag{28}$$

Using (27) twice in succession yields, after some algebra, the following condition on the z_i

$$\left[\frac{(\alpha z_i - 1)(bz_i - 1)(z_i - 1)^{M-1}}{z_i^L} - \alpha\beta\prod_{k=1}^{M}(1 - z_k)\right]\frac{1}{1 - z_i} = \left[\frac{(\alpha z_j - 1)(bz_j - 1)(z_j - 1)^{M-1}}{z_j^L} - \alpha\beta\prod_{k=1}^{M}(1 - z_k)\right]\frac{1}{1 - z_j}. \tag{29}$$

The wavefunction $\psi(x_1, \ldots x_M)$ corresponding to the largest eigenvalue $\lambda(\gamma)$ is invariant under translation, therefore

$$e^{\gamma}\alpha \prod_{k=1}^{M} z_k = 1. \tag{30}$$

One can rewrite the Bethe equations (29) in terms of two constants C, E as follows:

$$C = (-)^{M+1}\alpha\beta \prod_{k=1}^{M}(z_k - 1) \tag{31}$$

$$E = -\frac{1}{z_i - 1}\left[\frac{(\alpha z_i - 1)(bz_i - 1)(z_i - 1)^{M-1}}{z_i^L C} + 1\right]. \tag{32}$$

Under this form the Bethe equations (29) are much easier to solve. One first finds z_i the solutions of (32) (which depend on the unknown constants C and E). Then by inserting these solutions into (30) and (31), the constants C and E are determined. In appendix A, we show (see (A14), (A15) and (A19)) that, in so doing, the eigenvalue $\lambda(\gamma)$ can be written as

$$\lambda(\gamma) = -\sum_{n=1}^{\infty}\frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{dz}{2\pi i}\frac{1}{z^2}[Q(z)]^n \tag{33}$$

$$\gamma = -\sum_{n=1}^{\infty}\frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{dz}{2\pi i}\frac{1}{z}[Q(z)]^n \tag{34}$$

where

$$Q(z) = \frac{-z^L[1 + (z-1)E]}{(bz-1)(\alpha z - 1)(z-1)^{M-1}} \tag{35}$$

and the constant E is fixed by imposing

$$0 = \sum_{n=1}^{\infty}\frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{dz}{2\pi i}\frac{1}{z-1}[Q(z)]^n. \tag{36}$$

As is shown in appendix A the contours of integration in (33), (34) and (36) are small contours which surround 1 and $1/\alpha$ but do not surround $1/b$; the particular cases where $\alpha = 1$, $b = 1$ or $\alpha = b$ can be obtained easily as limiting cases since all the integrals which appear in the right-hand side of (33), (34) and (36) are rational functions of α and β.

Equations (33)–(36) determine the exact expression of $\lambda(\gamma)$ for arbitrary L, M, α and β. The difference between these equations and the corresponding equations of [25] is that in the present case we have an additional unknown constant E. This feature emerges from the structure of the Bethe equations (29).

5. Exact expressions for the velocity and diffusion constant

In principle, one can use (36) to expand E in powers of C. Replacing E by its expansion in powers of C in (33) and (34) gives the expansions of λ and γ in powers of C. Then one can eliminate C between the two expansions and this gives λ in powers of γ. This is what is done in this section to obtain exact expressions of the velocity and of the diffusion constant.

For example, to obtain the velocity v, one can note from (34) that C vanishes linearly with γ so that from (36), the limiting value $E(0)$ of E at $\gamma = 0$ is

$$E(0) = -\frac{X_{L,M}}{X_{L,M-1}} \tag{37}$$

where $X_{L,M}$ is defined by

$$X_{L,M} = \left[\oint_1 + \oint_{\frac{1}{\alpha}}\right] \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{z^L}{(z-1)^M} \frac{1}{(bz-1)(\alpha z-1)}. \tag{38}$$

Then from (33) and (34), one finds that for γ small $\lambda(\gamma) = v\gamma + \mathrm{O}(\gamma^2)$, with the velocity v given by

$$v = \frac{X_{L,M}X_{L-2,M-2} - X_{L,M-1}X_{L-2,M-1}}{Z_{L,M}} \tag{39}$$

where

$$Z_{L,M} = X_{L,M}X_{L-1,M-2} - X_{L,M-1}X_{L-1,M-1}. \tag{40}$$

Expression (39) may be simplified by using

$$X_{L,M} = X_{L-1,M} + X_{L-1,M-1} \tag{41}$$

to obtain

$$v = \frac{Z_{L-1,M} - Z_{L-1,M-1}}{Z_{L,M}}. \tag{42}$$

In a similar fashion one obtains from the second derivatives of (33), (34) and (36) at $\gamma = 0$, after a good deal of straightforward but tedious algebra,

$$\Delta = \frac{X_{L,M-1}}{Z_{L,M}^2}\{W_{2L,2M-1}X_{L-2,M-2} - W_{2L-2,2M-2}X_{L,M-1} \\ + v[W_{2L-1,2M-2}X_{L,M-1} - W_{2L,2M-1}X_{L-1,M-2}]\} \tag{43}$$

where $W_{2L,2M}$ is defined by

$$W_{2L,2M} = \left[\oint_1 + \oint_{\frac{1}{\alpha}}\right] \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{z^{2L}}{(z-1)^{2M}} \frac{[1+E(0)(z-1)]^2}{(bz-1)^2(\alpha z-1)^2}. \tag{44}$$

Expression (43) can be simplified by using (39)–(41) to obtain

$$\Delta = \frac{X_{L,M-1}^2}{Z_{L,M}^3}\{W_{2L,2M-1}Z_{L-1,M-1} - W_{2L-2,2M-2}Z_{L,M} \\ + W_{2L-1,2M-2}[Z_{L-1,M} - Z_{L-1,M-1}]\}. \tag{45}$$

Alternatively, one could obtain (45) directly from (33)–(36) by using, for example, `Mathematica`. The integrals in the above expressions can be evaluated by residues. In this way one can show that the integral expressions for $Z_{L,M}$ and v given by (38), (40) and (42) are equivalent to those derived in [15, 16] within the matrix product formulation. However, exact evaluation of the integrals involved in the diffusion constant (45) results, in general, in cumbersome expressions.

Remark. For the case of a second-class particle ($\alpha = \beta = 1$) simplification of (45) is possible and one recovers the expression first presented in [28] which was originally obtained using a matrix approach:

$$\Delta = 2\frac{(2L-3)!}{(2M-1)!(2L-2M+1)!}\left[\frac{(M-1)!(L-M)!}{(L-1)!}\right]^2 \\ \times[(L-5)(M-1)(L-M) + (L-1)(2L-1)]. \tag{46}$$

The derivation of (46) from (45) is tedious and not illuminating, therefore, we do not present it. In principle, the matrix approach could be extended to calculate Δ for general α and β [31] but such an expression for Δ has not been obtained due to the complexity of the calculation.

6. Asymptotics and phase diagram

In order to obtain the phase diagram it suffices to determine the asymptotic form of $Z_{L,M}$ which in turn determines the asymptotic form of the velocity (42). We carry this out in detail in appendix B, but would like to outline here how the different phases arise. We restrict ourselves to $\beta < 1$ ($b > 0$) and $\alpha < 1$.

Consider the quantity $X_{L,M}$ given by (38). In the limit of L, M large (with fixed $\rho = L/M$) there are three possible dominant contributions to the integral, all lying on the real axis: a saddle point at $z_c = 1/(1-\rho)$; a pole at $z = 1/b$ and a pole at $z = 1/\alpha$. The possible dominant and subdominant contributions to $X_{L,M}$ gives rise to four phases as follows.

(1) If $1/\alpha < z_c < 1/b$ the contours of the two integrals in (38) may be merged and deformed to pass through the saddle point. Therefore, only the saddle point contributes.
(2) If $1/\alpha < z_c$ and $1/b < z_c$ the contours of the two integrals may be merged and deformed to pass through the saddle point. However, the contour must make a clockwise detour around the pole at $z = 1/b$. Therefore, the pole at $z = 1/b$ is the dominant contribution and the saddle point is the subdominant contribution.
(3) If $1/\alpha > z_c$ and $1/b > z_c$ the two integrals give separate contributions. The pole at $z = 1/\alpha$ gives the dominant contribution and the integral around $z = 1$ may be deformed to pass through the saddle point and gives the subdominant contribution.
(4) If $1/\alpha > z_c > 1/b$ the two integrals give separate contributions: the pole at $z = 1/\alpha$ and the clockwise integral around the pole at $z = 1/b$.

In appendix B the dominant contributions to the desired integrals are evaluated and expressions (8)–(11) are established. At this point we can already see the interesting feature that since Z in (40) is a difference of products of X, the subdominant contribution as well as the dominant contribution to the integral X must be evaluated to obtain Z and the velocity. Also note that in phase where $1/\alpha < z_c < 1/b$, power law decays in correlation functions, for example the density profile, will arise from the saddle point being dominant. In the other phases a dominant pole will give rise to exponential decays. Of particular interest is the phase where $1/\alpha > z_c > 1/b$ and the two poles compete. As described in the introduction, this is the phase where a shock exists.

7. Scaling of the large deviation function for $1 - \alpha < \rho < \beta$

In this phase, because the integrals are dominated by the saddle point, the analysis of the asymptotics of the exact expression of $\lambda(\gamma)$ given by (33)–(36) is rather different from the other cases. In these expressions a contour integral actually implies two integrals around $z = 1$ and $z = 1/\alpha$ but in this phase, for large L, one expects all the integrals to be dominated by their saddle point $z_c = 1/(1-\rho)$. So, to lighten the notation we write a single integral. Let us replace the variables z and E in (33)–(36) by y and F

$$z = z_c + y \tag{47}$$

and

$$E = -\frac{1}{z_c - 1} + \frac{1}{z_c - 1}\frac{F}{L}. \tag{48}$$

Clearly, the values of y which contribute to the integrals in (33), (34) and (36) are of order $y = \mathrm{O}(L^{-1/2})$ so that one can rewrite (33), (34) and (36) as

$$\lambda(\gamma) = -\frac{1}{z_c^2} S_0 + \frac{2}{z_c^3} S_1 - \frac{3}{z_c^4} S_2 + \frac{4}{z_c^5} S_3 + \mathrm{O}\left(\frac{S_3}{L^{1/2}}\right) \tag{49}$$

$$\gamma = -\frac{1}{z_c}S_0 + \frac{1}{z_c^2}S_1 - \frac{1}{z_c^3}S_2 + \frac{1}{z_c^4}S_3 + \mathrm{O}\left(\frac{S_3}{L^{1/2}}\right) \tag{50}$$

$$0 = \frac{1}{z_c - 1}S_0 - \frac{1}{(z_c-1)^2}S_1 + \frac{1}{(z_c-1)^3}S_2 - \frac{1}{(z_c-1)^4}S_3 + \mathrm{O}\left(\frac{S_3}{L^{1/2}}\right) \tag{51}$$

where S_p is given by

$$S_p = \sum_{n\geqslant 1} \frac{C^n}{n} \oint \frac{\mathrm{d}y}{2\pi\mathrm{i}} \left[R(y)\left(\frac{-y}{z_c-1} + \frac{F}{L} + \frac{Fy}{L(z_c-1)}\right)\right]^n y^p \tag{52}$$

with

$$R(y) = \frac{1}{(1 - bz_c - by)(\alpha z_c + \alpha y - 1)} \frac{(z_c+y)^L}{(z_c+y-1)^{M-1}}. \tag{53}$$

Under the assumption (which we will check later) that F is of order one (in the large L limit), if we define

$$g(y) = \log(z_c + y) - \rho \log(z_c - 1 + y) \tag{54}$$

we can evaluate the leading orders of the integrals (52).

For p odd, the leading large L behaviour is given by

$$S_p \simeq \frac{(-)^{\frac{p+3}{2}}}{\sqrt{2\pi}} \frac{1-\rho}{\rho} \frac{D}{L^{1+\frac{p}{2}}} \left(\frac{1}{g''(0)}\right)^{1+\frac{p}{2}} p!! \tag{55}$$

where

$$D = C\mathrm{e}^{Lg(0)} \frac{1 - z_c}{(bz_c - 1)(\alpha z_c - 1)}. \tag{56}$$

For p even the leading order in the range where D is of order one is

$$\begin{aligned} S_p \simeq \frac{(-)^{\frac{p}{2}}}{\sqrt{2\pi}} \frac{D}{L^{\frac{p+3}{2}}} \left(\frac{1}{g''(0)}\right)^{\frac{p+5}{2}} \bigg\{ & Fg''(0)^2(p-1)!! \\ & + \frac{(1-\rho)^2}{\rho}\left[\frac{1}{\rho} - \frac{b}{\rho+b-1} - \frac{\alpha}{\alpha-1+\rho}\right] g''(0)(p+1)!! \\ & - \frac{1-\rho}{\rho}\frac{g'''(0)}{6}(p+3)!!\bigg\} \\ & + \frac{D^2}{2}\left(\frac{1-\rho}{\rho}\right)^2 \frac{1}{L^{\frac{p+3}{2}}} \left(\frac{1}{2g''(0)}\right)^{\frac{p+3}{2}} \frac{(-)^{\frac{p+2}{2}}}{\sqrt{2\pi}}(p+1)!! \end{aligned} \tag{57}$$

where we define $(p-1)!! = 1$ for $p = 0$. F is fixed through (51) by

$$S_1 \simeq (z_c - 1)S_0 \tag{58}$$

and from (49) and (50) we obtain

$$\gamma \simeq -\frac{1}{z_c^2(z_c-1)}S_1 \tag{59}$$

$$\lambda(\gamma) - \gamma\frac{2 - z_c}{z_c} \simeq \frac{1}{z_c^5(z_c-1)^2}[S_3(2 - 3z_c) - S_2 z_c(1 - z_c)]. \tag{60}$$

Using (55) and (57), (58) gives

$$F \simeq \frac{1}{(1-\rho)}\left[-\frac{1+\rho}{\rho} + \frac{b}{b-1+\rho} + \frac{\alpha}{\alpha-1+\rho}\right] + \frac{D}{\rho(1-\rho)2^{5/2}} \tag{61}$$

which is consistent with our earlier asumption that F is of order one. From (59) and (60) we find

$$\gamma = \frac{-D}{\sqrt{2\pi\rho(1-\rho)}L^{3/2}} \tag{62}$$

$$\lambda(\gamma) - \gamma(1-2\rho) \simeq \frac{2\gamma}{L}\left[2 - \rho\left(1 + \frac{1-\beta}{\rho-\beta} + \frac{\alpha}{\alpha-1+\rho}\right)\right] + \gamma^2 L^{1/2}\frac{\sqrt{\pi\rho(1-\rho)}}{8} \tag{63}$$

as announced in (12).

8. Discussion

In this paper we have shown how the Bethe ansatz can be used to calculate exactly via (33)–(36) the large deviation function of the displacement of the defect particle. By analysing the asymptotics of (33)–(36) we could recover the velocity and phase diagram [15, 16] of the asymmetric exclusion model with a moving defect. The approach also allows new results (such as all the cumulants of the displacement of the defect) to be obtained, in particular the diffusion constant of the defect particle in the various phases. This adds to the body of knowledge concerning diffusion constants within the asymmetric exclusion process. For example the exact expression for the diffusion constant of a first-class particle calculated in [20] allowed the determination of a universal amplitude for the centre of mass fluctuation for growth processes described by the one-dimensional KPZ equation [4]. The diffusion constant of a second-class particle is of interest since it is closely related to the motion of shocks. In [14] the diffusion constant for a second-class particle starting at the origin of an infinite lattice with a shock initial condition was calculated. Our results (11) for the phase exhibiting a shock ($\beta < \rho < 1-\alpha$) exactly agrees with that of [14]. This is of interest since it shows that a single defect can provoke a shock in the ring geometry with the same behaviour as a shock on the infinite line [33]. If the fluctuations of the shock on a ring with a defect are identical to the fluctuations of the shock on an infinite line, this means that our results (33)–(36) should give the whole large deviation function of a shock position on an infinite line. The behaviour of shocks and shock fluctuations is also connected to the phase diagram and density profile for systems with open boundary conditions [34].

When $\gamma \to 0$ the wavefunction (22) reduces to the steady state probabilities for each configuration. Therefore, in principle, the steady state of the system, previously constructed using a matrix product [6,15,16], can be extracted from the present Bethe ansatz (22) by taking the limit $\gamma \to 0$. This shows that a coordinate Bethe ansatz is capable of describing non-trivial steady states of stochastic systems. In particular, it would be interesting to understand further how this works and to see if the approach might be generalizable to larger numbers of species. The matrix product steady state of the present model is very closely related to that of the ASEP with open boundary conditions [6,18]. It would be of great interest to determine whether some implementation of the Bethe ansatz, perhaps related to that of the present work, could be used to recover the steady state with open boundary conditions. A major difficulty in doing so is that the particle number is not conserved with open boundaries.

Returning to the case of a second-class particle, it is of interest to review how its dynamics are related to the spreading of excess mass. The central idea, termed coupling [1], is well known in the mathematical community but less so within physics. Consider two systems containing only first-class particles, identical except that one system has M particles and the other $M-1$ particles. The two systems start from initial conditions differing only by the position of the extra particle in the system with M particles. In order to implement the dynamics one can consider at each time step randomly choosing a pair of sites $i, i+1$ to update; then if there is particle at site i and a hole at site $i+1$ the particle is moved forward. In the dynamics let us choose the same pairs of sites in the two systems at each update (one can think of using the same random numbers in a Monte Carlo program). Now it is easy to convince oneself that after any length of time the configurations of the two systems will differ only by the position of the extra particle (note that if we label the particles, the label of the extra particle will change under the dynamics). Further, one can convince oneself that the position of the extra particle has precisely the dynamics of a second-class particle in the ASEP. Conversely, the system comprising $M-1$ first-class particles and one second-class particle that we have studied describes the motion of an extra particle added to a system of $M-1$ particles. Therefore, the diffusion constant of the second-class particle we have calculated here serves to describe the spreading of excess mass in the ASEP.

Approximate calculations such as mode coupling [29, 32] have led to the following understanding of the motion of excess mass fluctuations: the drift speed is $1-2\rho$ as in (8) for $\alpha=\beta=1$ and the spreading of density fluctutations around the drift grows as $t^{2/3}$ on an infinite system i.e. it is superdiffusive. This superdiffusive motion can be recovered from the $L^{1/2}$ finite system size dependence (8) of the diffusion constant of a second-class particle [28] if we assume that a scaling form holds and the variance of the distance travelled by the second-class particle can be written as

$$\langle y_t^2\rangle - \langle y_t\rangle^2 \sim tL^{1/2} f(t/L^z) \tag{64}$$

where z is the dynamic exponent and $f(x)$ is a scaling function tending to a constant as $x\to\infty$. Now the dynamic exponent for the ASEP is known by the Bethe ansatz to be $z=\frac{3}{2}$ [23,24] and we expect the same exponent in the present model. In the limit $L\to\infty$ for large but fixed t, the variance $\langle y_t^2\rangle-\langle y_t\rangle^2$ should not depend on system size therefore the scaling function must obey $f(x)\sim x^{1/2z}$ as $x\to 0$. We then find in this infinite system limit that $\langle y_t^2\rangle-\langle y_t\rangle^2\sim t^{4/3}$ so that the typical spread of density fluctuations grows as $t^{2/3}$. The spreading of mass fluctuations is also related to the scaling length $\xi\sim t^{2/3}$ of the KPZ equation in one dimension (see [4] for detailed discussion).

Finally, let us mention that one can easily extend the calculation of this paper to calculate the joint distribution of the distance y_t covered by the defect particle and of the total distance Y_t covered by all the first-class particles. One can show that

$$\lambda(\gamma,\delta) = \lim_{t\to\infty}\frac{\ln[\langle \mathrm{e}^{\gamma y_t+\delta Y_t}\rangle]}{t} \tag{65}$$

is still given by (23) for arbitrary L and M where the z_i and the constants C and E satisfy:

$$\mathrm{e}^{\gamma+(M-1)\delta}\alpha\prod_{k=1}^{M} z_k = 1 \tag{66}$$

$$C = (-)^{M+1}\alpha\beta\mathrm{e}^{\delta L}\prod_{k=1}^{M}(z_k-1) \tag{67}$$

instead of (30) and (31) with (32) unchanged.

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Appendix A. Analysis of the Bethe ansatz equations

The solution for $\{z_i\}$ of (30)–(32) which gives $\lambda \to 0$ as $\gamma \to 0$ is of the form $z_1 \to 1/\alpha$ and $z_k \to 1$ for $2 \leqslant k \leqslant M$. We analyse separately the cases $\alpha \neq 1$ and $\alpha = 1$ and for simplicity assume $\beta \neq 1$ and $\beta \neq \alpha$ although there is no problem in extending the analysis to include these cases.

Case $\alpha \neq 1$. Consider the root z_1 and the $M-1$ roots z_k for $2 \leqslant k \leqslant M$ of (32) which we rewrite as

$$(z-1)^{M-1}(bz-1)(\alpha z-1) + z^L C[1+(z-1)E] = 0 \tag{A1}$$

such that $z_1 \to 1/\alpha$ and $z_k \to 1$ as $C \to 0$. Define

$$R(z) = \frac{-z^L[1+(z-1)E]}{(bz-1)(\alpha z-1)} \tag{A2}$$

then if z_k is a root of (A1) such that $z_k \to 1$ as $C \to 0$ one has for small C

$$z_k = 1 + [C\mathrm{e}^{2\mathrm{i}\pi k} R(z_k)]^{\frac{1}{M-1}}. \tag{A3}$$

We wish to calculate expressions (23), (30) and (31) of the form $\sum_k h(z_k)$ (e.g. equation (23) where $h = 1/z$). If $h(z)$ is analytic near $z = 1$, one has by the residue theorem

$$h(z_k) = \oint_1 \frac{\mathrm{d}z}{2\pi\mathrm{i}} h(z) \frac{1 - [C\mathrm{e}^{2\mathrm{i}\pi k} R(z)]^{\frac{1}{M-1}} R'(z)/[(M-1)R(z)]}{z - 1 - [C\mathrm{e}^{2\mathrm{i}\pi k} R(z)]^{\frac{1}{M-1}}} \tag{A4}$$

where the contour is a circle centred on one and of radius ϵ with $|C|^{\frac{1}{M-1}} \ll \epsilon \ll 1$. (To understand (A4) notice that the numerator is just the derivative of the denominator.) Expanding in powers of $C^{\frac{1}{M-1}}$ and after an integration by parts, this gives

$$h(z_k) = h(1) + \sum_{p=1}^{\infty} \frac{1}{p} [C\mathrm{e}^{2\mathrm{i}\pi k}]^{\frac{p}{M-1}} \oint_1 \frac{\mathrm{d}z}{2\pi\mathrm{i}} h'(z) \frac{[R(z)]^{\frac{p}{M-1}}}{(z-1)^p}. \tag{A5}$$

Then summing over the roots $2 \leqslant k \leqslant M$ leads to

$$\sum_{k=2}^{M} h(z_k) = (M-1)h(1) + \sum_{n=1}^{\infty} \frac{1}{n} C^n \oint_1 \frac{\mathrm{d}z}{2\pi\mathrm{i}} h'(z) \frac{[R(z)]^n}{(z-1)^{n(M-1)}}. \tag{A6}$$

Similarly, if $h(z)$ is analytic near $z = 1/\alpha$ and we define

$$S(z) = \frac{-z^L[1+(z-1)E]}{\alpha(bz-1)(z-1)^{M-1}} \tag{A7}$$

then

$$h(z_1) = \oint_{1/\alpha} \frac{\mathrm{d}z}{2\pi\mathrm{i}} h(z) \frac{1 - CS'(z)}{z - \frac{1}{\alpha} - CS(z)} \tag{A8}$$

where the contour is a circle centred on $1/\alpha$ and of radius ϵ with $|C| \ll \epsilon \ll 1$. After expanding in powers of C and an integration by parts, this gives

$$h(z_1) = h\left(\frac{1}{\alpha}\right) + \sum_{n=1}^{\infty} \frac{C^n}{n} \oint_{\frac{1}{\alpha}} \frac{\mathrm{d}z}{2\pi\mathrm{i}} h'(z) \frac{[S(z)]^n}{(z-\frac{1}{\alpha})^n}. \tag{A9}$$

Therefore, if one defines $Q(z)$ by

$$Q(z) = \frac{-z^L[1+(z-1)E]}{(bz-1)(\alpha z-1)(z-1)^{M-1}} = \frac{R(z)}{(z-1)^{M-1}} = \frac{S(z)}{z-\frac{1}{\alpha}} \tag{A10}$$

one finds by combining (A9) and (A6)

$$\sum_{k=1}^{M} h(z_k) = (M-1)h(1) + h\left(\frac{1}{\alpha}\right) + \sum_{n=1}^{\infty} \frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{\mathrm{d}z}{2\pi \mathrm{i}} h'(z)[Q(z)]^n. \tag{A11}$$

Writing (23) and (30) as

$$\lambda(\gamma) = -(M-1+\alpha) + \sum_{k=1}^{M} \frac{1}{z_k} \tag{A12}$$

$$\gamma = -\log\alpha - \sum_{k=1}^{M} \log z_k \tag{A13}$$

one finds that

$$\lambda(\gamma) = -\sum_{n=1}^{\infty} \frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{\mathrm{d}z}{2\pi \mathrm{i}}\frac{1}{z^2}[Q(z)]^n \tag{A14}$$

$$\gamma = -\sum_{n=1}^{\infty} \frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{\mathrm{d}z}{2\pi \mathrm{i}}\frac{1}{z}[Q(z)]^n \tag{A15}$$

where $Q(z)$ is given by (A10). Then, with the use of (A3), replacing (31) by

$$(1-z_1)\prod_{k=2}^{M}[R(z_k)]^{\frac{1}{M-1}} = \frac{1}{\alpha\beta} \tag{A16}$$

and using the fact (A6) and (A9) that

$$0 = \ln(\alpha\beta) + \ln(1-z_1) + \frac{1}{M-1}\sum_{k=2}^{M} \ln R(z_k) \tag{A17}$$

$$= \sum_{n=1}^{\infty} \frac{C^n}{n}\frac{1}{2\pi \mathrm{i}}\left[\frac{1}{M-1}\oint_1 \mathrm{d}z\, \frac{R'(z)[R(z)]^{n-1}}{(z-1)^{n(M-1)}} + \oint_{\frac{1}{\alpha}} \mathrm{d}z\, \frac{1}{z-1}\frac{[S(z)]^n}{(z-\frac{1}{\alpha})^n}\right] \tag{A18}$$

one finds that (31) is satisfied if

$$0 = \sum_{n=1}^{\infty} \frac{C^n}{n}\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right]\frac{\mathrm{d}z}{2\pi \mathrm{i}}\frac{1}{z-1}[Q(z)]^n. \tag{A19}$$

Case $\alpha = 1$. Let

$$P(z) = \frac{-z^L[1+(z-1)E]}{(bz-1)}. \tag{A20}$$

Then if z_k is the root such that $z_k \to 1$ as $C \to 0$ with for small C

$$z_k = 1 + [C\mathrm{e}^{2\mathrm{i}\pi k}P(z_k)]^{\frac{1}{M}} \tag{A21}$$

and if $h(z)$ is analytic near $z = 1$, one has

$$h(z_k) = \oint_1 \frac{\mathrm{d}z}{2\pi \mathrm{i}} h(z)\frac{1-[C\mathrm{e}^{2\mathrm{i}\pi k}P(z)]^{\frac{1}{M}}P'(z)/[MP(z)]}{z-1-[C\mathrm{e}^{2\mathrm{i}\pi k}P(z)]^{\frac{1}{M}}}. \tag{A22}$$

Then summing over the roots $0 \leqslant k \leqslant M-1$ leads to

$$\sum_{k=0}^{M-1} h(z_k) = Mh(1) + \sum_{n=1}^{\infty}\frac{1}{n}C^n\oint_1 \frac{\mathrm{d}z}{2\pi \mathrm{i}} h'(z)\frac{[P(z)]^n}{(z-1)^{nM}}. \tag{A23}$$

Therefore, the equations for case $\alpha = 1$ are given by exactly the same expressions as the case $\alpha \neq 1$ (33), (34) and (36) with the replacement

$$\left[\oint_1 + \oint_{\frac{1}{\alpha}}\right] \to \oint_1.$$

Appendix B. Asymptotic evaluation of velocity and diffusion constant

Evaluation of the velocity

For $1/\alpha < z_c$ *and* $1/b > z_c$. In this phase (38) is dominated by $S_{L,M}$ the saddle point contribution

$$X_{L,M} = S_{L,M} + \mathrm{O}(S_{L,M}/L) \tag{B1}$$

where

$$S_{L,M} = \frac{1}{\sqrt{2\pi L}} \frac{[\rho(1-\rho)]^{1/2}}{(b+\rho-1)(\alpha+\rho-1)} \frac{z_c^L}{(z_c-1)^M}. \tag{B2}$$

However, the leading contributions to $X_{L,M}$ cancel in (40). To evaluate the next leading contribution we write $Z_{L,M}$ as a double integral using (38)

$$Z_{L,M} = \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{1}{(bz-1)(\alpha z-1)} \oint \frac{\mathrm{d}\tilde{z}}{2\pi \mathrm{i}} \frac{1}{(b\tilde{z}-1)(\alpha\tilde{z}-1)} \frac{z^L}{(z-1)^M} \frac{\tilde{z}^L}{(\tilde{z}-1)^M} \times \frac{(\tilde{z}-1)(\tilde{z}-z)}{\tilde{z}}. \tag{B3}$$

The double integral is dominated by the saddle point $z = \tilde{z} = z_c = 1/(1-\rho)$ and can be evaluated to be

$$Z_{L,M} \simeq \frac{\rho S_{L,M}^2}{(1-\rho)L}. \tag{B4}$$

From (42) one obtains $v = 1/z_c - (z_c-1)/z_c$, so that

$$v = 1 - 2\rho \tag{B5}$$

as in (8).

For $1/\alpha < z_c$ *and* $1/b < z_c$. As explained in section 6, in this phase the dominant contribution to (38) is the pole at $1/b$ and the saddle point is subdominant:

$$X_{L,M} = B_{L,M} + S_{L,M} + \mathrm{O}(S_{L,M}/L) \tag{B6}$$

where B represents the contribution of the clockwise contour around the pole $z = 1/b$

$$B_{L,M} = \frac{1}{b-\alpha} \frac{1}{(1-b)^M b^{L-M}}. \tag{B7}$$

Therefore, from (40)

$$Z_{L,M} \simeq \frac{(1-bz_c)^2}{bz_c} B_{L,M} S_{L,M} \tag{B8}$$

and from (42)

$$v = 1 - \beta - \rho \tag{B9}$$

as in (9).

For $1/\alpha > z_c$ *and* $1/b > z_c$. In this phase the pole at $1/\alpha$ is the dominant contribution to (38) and the saddle point is subdominant

$$X_{L,M} = A_{L,M} + S_{L,M} + \mathrm{O}(S_{L,M}/L) \tag{B10}$$

where $A_{L,M}$ is given by

$$A_{L,M} = \frac{1}{b-\alpha}\frac{1}{(1-\alpha)^M\alpha^{L-M}}. \tag{B11}$$

$Z_{L,M}$ may be determined by symmetry considerations from the previous phase: under interchange of α and b (B6) becomes (B10) and (B8) becomes

$$Z_{L,M} \simeq \frac{(1-\alpha z_c)^2}{\alpha z_c} A_{L,M} S_{L,M} \tag{B12}$$

and we find

$$v = \alpha - \rho \tag{B13}$$

as in (10).

For $1/\alpha > z_c$ *and* $1/b < z_c$. In this phase

$$X_{L,M} \simeq A_{L,M} + B_{L,M} + \mathrm{O}(S_{L,M}) \tag{B14}$$

so that

$$Z_{L,M} \simeq \frac{(b-\alpha)^2}{b\alpha} A_{L,M} B_{L,M} \tag{B15}$$

and

$$v = \alpha - \beta \tag{B16}$$

as in (11).

Evaluation of the diffusion constant

In order to compute the diffusion constant given by (45)

$$\Delta = \frac{X^2_{L,M-1}}{Z^3_{L,M}} U_{L,M} \tag{B17}$$

where

$$U_{L,M} = W_{2L,2M-1} Z_{L-1,M-1} + W_{2L-1,2M-2}(Z_{L-1,M} - Z_{L-1,M-1}) - W_{2L-2,2M-2} Z_{L,M} \tag{B18}$$

we need first to evaluate the asymptotics of $U_{L,M}$. Using the integral definitions (44) and (B3) we may write (B18) as

$$U_{L,M} = \oint \frac{\mathrm{d}w}{2\pi \mathrm{i}} \frac{w^{2L}}{(w-1)^{2M}} \frac{[1+E(0)(w-1)]^2}{(bw-1)^2(\alpha w-1)^2} \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{z^L}{(z-1)^M} \frac{1}{(bz-1)(\alpha z-1)}$$
$$\times \oint \frac{\mathrm{d}\tilde{z}}{2\pi \mathrm{i}} \frac{\tilde{z}^L}{(\tilde{z}-1)^M} \frac{(\tilde{z}-1)(\tilde{z}-z)}{(b\tilde{z}-1)(\alpha\tilde{z}-1)} \frac{w-1}{w^2} \frac{w-z}{z} \frac{w-\tilde{z}}{\tilde{z}^2}. \tag{B19}$$

For $1/\alpha > z_c$ *and* $1/b > z_c$. In this phase all integrations are dominated by their saddle points. However, care is required to correctly identify the first non-vanishing contribution to (B19). This is done most systematically by considering the scaling of the large deviation function and we carry this out in section 7 where we show

$$\Delta \simeq \frac{(L\pi\rho(1-\rho))^{1/2}}{4}. \tag{B20}$$

For $1/\alpha < z_c$ *and* $1/b < z_c$. To evaluate (B19) we carry out the integrals in sequence. In the first integral over $\tilde{z}$ we keep an *apparently* subdominant term (proportional to $S_{L,M}$) as well the term proportional to $B_{L,M}$, because when we integrate over z we find both terms give leading contributions proportional to $S_{L,M}B_{L,M}$ i.e. the dominant contributions to the triple integral come from w at the pole, one of $z, \tilde{z}$ at the pole and the other at the saddle point:

$$\begin{aligned}
U_{L,M} &\simeq \oint \frac{\mathrm{d}w}{2\pi \mathrm{i}} \frac{w^{2L-2}}{(w-1)^{2M-1}} \frac{[1+E(0)(w-1)]^2}{(bw-1)^2(\alpha w-1)^2} \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{z^L}{(z-1)^M} \frac{1}{(bz-1)(\alpha z-1)} \\
&\quad \times \left[B_{L,M} \frac{(b-1)(bw-1)(w-z)(bz-1)}{bz} \right. \\
&\quad \left. + S_{L,M} \frac{(z_c-1)(w-z_c)(w-z)(z_c-z)}{z_c^2 z} \right] \\
&\simeq \oint \frac{\mathrm{d}w}{2\pi \mathrm{i}} \frac{w^{2L-2}}{(w-1)^{2M-1}} \frac{[1+E(0)(w-1)]^2}{(bw-1)^2(\alpha w-1)^2} S_{L,M} B_{L,M} \\
&\quad \times \left[\frac{(b-1)(bw-1)(w-z_c)(bz_c-1)}{bz_c} \right. \\
&\quad \left. + \frac{(z_c-1)(w-z_c)(bw-1)(bz_c-1)}{bz_c^2} \right] \\
&= S_{L,M} B_{L,M} \frac{(bz_c-1)^2}{bz_c^2} \oint \frac{\mathrm{d}w}{2\pi \mathrm{i}} \frac{w^{2L-2}}{(w-1)^{2M-1}} \frac{[1+E(0)(w-1)]^2 (w-z_c)}{(bw-1)(\alpha w-1)^2} \\
&\simeq S_{L,M} B_{L,M}^3 \frac{(1-b)(bz_c-1)^3}{z_c^2} \left[1 + E(0) \left(\frac{1-b}{b} \right) \right]^2.
\end{aligned} \tag{B21}$$

In this phase the behaviour (B6) and the form of (B7) and (B2) imply that $E(0)$ given by (37) becomes

$$E(0) \simeq -\frac{b}{1-b} \left[1 + \frac{(1-bz_c)}{(1-b)} \frac{S_{L,M}}{B_{L,M}} \right]. \tag{B22}$$

Therefore

$$U_{L,M} \simeq S_{L,M}^3 B_{L,M} \frac{(bz_c-1)^5}{z_c^2(1-b)} \tag{B23}$$

and (B17) along with (B8) and (B6) and $b = 1-\beta$, yields

$$\Delta \simeq \frac{\beta(1-\beta)}{\rho-\beta} \tag{B24}$$

as in (9).

For $1/\alpha > z_c$ *and* $1/b > z_c$. For this phase the evaluation of the integral (B19) is very similar to that outlined above for the previous phase, with α replacing b. In carrying out the final integral over w a factor of -1 is introduced due to the opposite directions of the integral around $1/\alpha$ and $1/b$. Therefore, one obtains the diffusion constant by interchanging β and $1-\alpha$ in (B24) and multiplying by -1

$$\Delta \simeq \frac{\alpha(1-\alpha)}{1-\rho-\alpha} \tag{B25}$$

as in (10).

For $1/\alpha > z_c$ *and* $1/b < z_c$. In this phase it turns out that the dominant contributions to $U_{L,M}$ come from one of $z, \tilde{z}$ at the pole $1/b$ and the other at the pole $1/\alpha$ and w at either of the two poles. Carrying out the integrals in (B19) in sequence gives

$$\begin{aligned} U_{L,M} \simeq & \oint \frac{\mathrm{d}w}{2\pi \mathrm{i}} \frac{w^{2L-2}}{(w-1)^{2M-1}} \frac{[1+E(0)(w-1)]^2}{(bw-1)^2(\alpha w-1)^2} \oint \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{z^L}{(z-1)^M} \\ & \times \left[A_{L,M} \frac{(\alpha-1)(w-z)(\alpha w-1)}{\alpha(bz-1)z} + B_{L,M} \frac{(b-1)(w-z)(bw-1)}{b(\alpha z-1)z} \right] \\ \simeq & A_{L,M} B_{L,M} \frac{(b-\alpha)^2}{\alpha b} \oint \frac{\mathrm{d}w}{2\pi \mathrm{i}} \frac{w^{2L-2}}{(w-1)^{2M-1}} \frac{[1+E(0)(w-1)]^2}{(bw-1)(\alpha w-1)} \\ \simeq & A_{L,M} B_{L,M}^3 \frac{(b-\alpha)^3(1-b)}{\alpha} \left[1 + E(0) \left(\frac{1-b}{b} \right) \right]^2 \\ & + A_{L,M}^3 B_{L,M} \frac{(b-\alpha)^3(1-\alpha)}{b} \left[1 + E(0) \left(\frac{1-\alpha}{\alpha} \right) \right]^2 . \end{aligned} \tag{B26}$$

First consider $B_{L,M} \gg A_{L,M}$. Then due to the form of $X_{L,M}$ (B14) in this phase one has

$$E(0) \simeq -\frac{b}{1-b} \left[1 + \frac{(\alpha-b)}{(1-b)\alpha} \frac{A_{L,M}}{B_{L,M}} \right]. \tag{B27}$$

Both terms in (B26) contribute and one obtains

$$U_{L,M} \simeq A_{L,M}^3 B_{L,M} \frac{(b-\alpha)^5}{\alpha^3 b(1-b)^2} [b(1-b) + \alpha(1-\alpha)]. \tag{B28}$$

Then (B14), (B15) and (B17) imply

$$\Delta \simeq \frac{\beta(1-\beta) + \alpha(1-\alpha)}{1-\beta-\alpha} \tag{B29}$$

as in (11).

In the case where $A_{L,M} \gg B_{L,M}$

$$E(0) \simeq -\frac{\alpha}{1-\alpha} \left[1 + \frac{(b-\alpha)}{b(1-\alpha)} \frac{B_{L,M}}{A_{L,M}} \right] \tag{B30}$$

however, it turns out that one obtains the same expression for the diffusion constant (B29).

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