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A matrix ansatz for the diffusion of an impurity in the asymmetric exclusion process

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Abstract
We study the fluctuations of the position of an impurity in the asymmetric exclusion process on a ring with an arbitrary number of particles and holes. The steady state of this model is exactly known and four different phases appear in the limit of a large system. We calculate the diffusion constant of the impurity by using a matrix product method and also obtain a representation for unequal time correlation functions. We show that our results found by the matrix ansatz agree with those obtained previously by the Bethe ansatz.

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1. Introduction

The one-dimensional asymmetric simple exclusion process (ASEP) is a model of driven diffusive particles on a lattice with hard-core exclusion. The ASEP appears as a minimal building block in different models that describe a large variety of physical phenomena such as growth processes (the ASEP is a discrete version of the KPZ equation [1]), hopping conductivity [2], diffusion of particles through narrow pores, polymer reptation and traffic flow [3–5]. From a theoretical point of view the ASEP, as a member of the class of driven diffusive particle systems [6, 7], is a key model for the study of non-equilibrium statistical mechanics. In particular, it is one of the very few systems, far from equilibrium, for which exact solutions have been obtained and a large body of knowledge has been gathered in the last decade (for recent reviews, see [8, 9]). The ASEP can be studied with the help of many different methods ranging from probability theory [10, 11] to integrable systems techniques [12, 13] and random matrix theory [14].

A breakthrough in the study of the ASEP resulted from the introduction of the 'matrix product ansatz' [15] in which steady-state weights are expressed as matrix elements. With this technique, many steady-state properties such as the current, the density profile and non-equilibrium analogues to the free energy [16] can be exactly calculated. Due to its algebraic character, this method has also triggered the study of diffusion algebras that appear in general reaction–diffusion processes [17, 18]. These exact calculations provide a quantitative understanding of a large range of phenomena such as non-equilibrium phase transitions, symmetry breaking in one dimension [19], travelling and diffusing shocks [20] etc. The matrix product ansatz has also been used to calculate steady states for exclusion processes with second-class [21–23] and third-class particles [24]. The introduction of different species of particles allows us to localize a shock [25] (it corresponds mathematically to coupling identical systems [26]).

The presence of a defect in the ASEP can generate a shock dynamically. For example, a defective bond can induce a separation between a dense phase and a fluid phase [27]. However, such a model has not been solved analytically. A moving impurity may also induce a shock in the stationary state [29, 30]. A traffic-flow picture illustrates this fact: if particles represent cars and the defect a truck (which moves at a slow speed and is hard to overtake), then the shock corresponds to a traffic jam. The phase transition to a shock can also be interpreted as a dynamical version of Bose–Einstein condensation [28]. The position of the shock can be identified as the position of the truck itself; as such the location of the truck is a random variable that carries statistical information on the whole ensemble of particles. For example, the mean value of the location of the truck grows linearly with time, at long times, and thus allows us to define a mean velocity v of the truck. This scalar quantity v can be chosen as an order parameter: in the limit of large systems, changes in the analytic behaviour of v characterize phase transitions and allow us to define a phase diagram.

In this work, we study the fluctuations of the position of the shock in a system with a moving impurity around its mean value and calculate the associated diffusion constant. The diffusion constant is related to unequal time correlation functions in the stationary state. We shall obtain an explicit expression for these correlation functions. The diffusion constant has been found using the Bethe ansatz in [34]. However, the correlation functions, which are formally a linear combination of eigenvectors, have not been calculated from the Bethe ansatz. We show that the diffusion constant of an impurity can be calculated by a generalization of the matrix ansatz method that involves a suitable quadratic algebra. Our method generalizes the techniques used in [31–33] to study the diffusion of a tracer. The expressions we obtain can be identified with those derived using the Bethe ansatz.

The plan of this paper is as follows. In section 2, we define the model, discuss the properties of the steady state, describe the matrix ansatz for the stationary probabilities, recall the phase diagram, and derive a formal expression for the diffusion constant Δ in terms of some generalized weights. In section 3, we find a matrix ansatz for the generalized weights with the help of a new quadratic algebra and through a suitable regularization of the traces of this algebra. This allows us to express Δ as a linear combination of traces. In section 4, we calculate these traces and obtain a formula for the diffusion constant. Section 5 is devoted to a physical discussion of the properties of Δ in different parts of the phase diagram, and of the relation between the generalized weights and unequal time correlation functions. Concluding remarks appear in section 6. The appendices contain some useful mathematical identities and some derivations used in the main text.

2. The stationary state

We consider the model that was introduced and studied in [29, 30]. This model is defined on a ring of $L+1$ sites, numbered from 0 to L, with P particles (denoted by 1) and one impurity (denoted by 2) that hops with rate $\alpha \leqslant 1$ and can be overtaken by other particles with rate $\beta \leqslant 1$. Each site i is either occupied by a normal particle or by the impurity, or it is empty. Stochastic dynamical rules govern the evolution of the system and during the infinitesimal time step $\mathrm{d}t$, a bond $(i, i+1)$, with $0 \leqslant i \leqslant L$, evolves as follows,

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

where an empty site is represented by 0. All other transitions are forbidden. These rules define a Markov process and the evolution of the system is governed by the master equation

$$\frac{\mathrm{d}P_t(\mathcal{C}|\mathcal{C}_0)}{\mathrm{d}t} = \sum_{\mathcal{C}'} \mathcal{M}(C, C')P_t(\mathcal{C}'|\mathcal{C}_0). \tag{2}$$

Here $\mathcal{C}_0$ is the initial configuration and the Markov (or the incidence) matrix $\mathcal{M}(C, C^{'})$ encodes the transition rates between configurations. We shall work in the relative frame of the impurity unless the contrary is specified, i.e. we use the translation invariance of the system to relabel the sites, so that the impurity always remains on site number 0. The system has thus $\binom{L}{P} = \frac{L!}{P!(L-P)!}$ configurations.

In the long time limit, the system reaches a stationary state in which each configuration $\mathcal{C}$ has a stationary probability (or weight) $p(\mathcal{C})$. The stationary weights are solutions of the stationary master equation,

$$\sum_{\mathcal{C}'} \mathcal{M}(C, C')p(\mathcal{C}') = 0. \tag{3}$$

2.1. *Matrix ansatz for the stationary probabilities*

The computation of the stationary probabilities is non-trivial. As shown in [29, 30], $p(\mathcal{C})$ can be expressed as a trace of a matrix product involving non-commuting operators D, E and A,

$$p(\mathcal{C}) = \frac{1}{Z_{L,P}} \mathrm{Tr}\left(A\prod_{i=1}^{L}(\tau_i D + (1-\tau_i)E)\right) \tag{4}$$

where $\tau_i(\mathcal{C}) = 1$ if site i is occupied by a particle in the configuration $\mathcal{C}$ and $\tau_i(\mathcal{C}) = 0$ if it is empty. The normalization factor $Z_{L,P}$ ensures that the sum of all probabilities is equal to 1.

The matrices D, E and A satisfy the following algebra:

$$DE = D + E \qquad DA = \frac{1}{\beta}A \qquad AE = \frac{1}{\alpha}A. \tag{5}$$

These matrices have to be infinite dimensional unless $\alpha + \beta = 1$ [15]. A suitable representation of algebra (5) is

$$D = \begin{pmatrix} 1 & 1 & 0 & 0 & . & . \\ 0 & 1 & 1 & 0 & & \\ 0 & 0 & 1 & 1 & & \\ 0 & 0 & 0 & 1 & . & \\ . & & & & . & . \\ . & & & & & . \end{pmatrix} \qquad E = \begin{pmatrix} 1 & 0 & 0 & 0 & . & . \\ 1 & 1 & 0 & 0 & & \\ 0 & 1 & 1 & 0 & & \\ 0 & 0 & 1 & 1 & & \\ . & & & & . & . \\ . & & & & . & . \end{pmatrix} \qquad A = |\beta\rangle\langle\alpha| \tag{6}$$

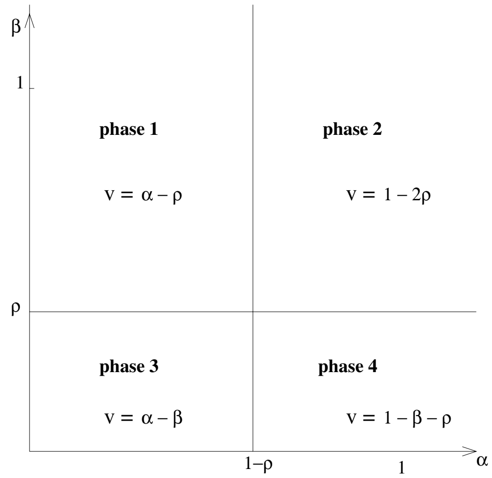

Figure 1. The phase diagram of the ASEP with an impurity.

where

$$\langle\alpha| = \kappa\left(1, \frac{1-\alpha}{\alpha}, \left(\frac{1-\alpha}{\alpha}\right)^2, \ldots\right) \qquad |\beta\rangle = \kappa\begin{pmatrix}1\\ \frac{1-\beta}{\beta}\\ \left(\frac{1-\beta}{\beta}\right)^2\\ \vdots\end{pmatrix} \qquad \text{with} \quad \kappa^2 = \frac{\alpha+\beta-1}{\alpha\beta}. \tag{7}$$

2.2. The phase diagram

The phase diagram is obtained in the large system limit, $L \to \infty$, while keeping the density P/L of the particles constant [30]. We recall briefly the results derived in [29, 30]. There are four principal phases. Transitions between different phases are characterized by non-analytic behaviour of the speed v of the impurity (in the reference frame of the lattice) and of the current J of the particles. Divergent correlation lengths are associated with the transitions. The speed of the impurity can be expressed in terms of the normalization factor [30]

$$v = \frac{Z_{L-1,P} - Z_{L-1,P-1}}{Z_{L,P}}. \tag{8}$$

The four phases are described as follows (see figure 1):

- For $\rho < \beta$ and $\rho < 1-\alpha$, the defect behaves essentially as a hole with $J = \rho(1-\rho)$ and $v = \alpha - \rho$.
- For $\beta < \rho$ and $1-\alpha < \rho$, the defect behaves essentially as a normal particle and $J = \rho(1-\rho)$ and $v = 1-\beta-\rho$.
- For $1-\alpha < \rho < \beta$, the defect is similar to a second class particle [21]; the density profile is uniform and the defect lowers the average speed of the particles. One has $J = \rho(1-\rho)$ and $v = 1-2\rho$.

- For $\beta < \rho < 1-\alpha$, the density profile presents a shock; the particles cannot easily overtake the defect and are blocked behind it. A single local defect induces a global phase separation in the system. Here, $J = \rho(\alpha-\beta)+\beta(1-\alpha)$ and $v = \alpha-\beta$.

2.3. Calculation of the normalization factor

The phase diagram was obtained in [30] from an asymptotic analysis of the normalization factor $Z_{L,P}$ defined in equation (4). This factor can also be expressed as a trace,

$$Z_{L,P} = \mathrm{Tr}(AG_{L,P}) = \langle\alpha|G_{L,P}|\beta\rangle \tag{9}$$

where $G_{L,P}$ is the sum of all matrices formed by multiplying P matrices D and $(L-P)$ matrices E in all possible orders, i.e.

$$G_{L,P} = \sum_{\tau_i=0,1} \delta\left(P - \sum_{i=1}^{L}\tau_i\right)\prod_{i=1}^{L}(\tau_i D + (1-\tau_i)E). \tag{10}$$

The matrix elements of $G_{L,P}$ are [30, 31]

$$\langle x'|G_{L,P}|x\rangle = \binom{L}{P}\binom{L}{P+x'-x} - \binom{L}{P+x'}\binom{L}{P-x}. \tag{11}$$

The normalization factor $Z_{L,P}$ can be calculated using these matrix elements as follows [30]. Starting from equation (9), we find

$$\frac{Z_{L,P}}{\kappa^2} = \sum_{x',x=1}^{\infty} a^{x'-1}b^{x-1}\binom{L}{P}\binom{L}{P+x'-x} - a^{x'-1}\binom{L}{P+x'}b^{x-1}\binom{L}{P-x} \tag{12}$$

where we have defined

$$a = \frac{1-\alpha}{\alpha} \quad \text{and} \quad b = \frac{1-\beta}{\beta}. \tag{13}$$

We now introduce polynomial functions that generalize the binomial coefficients. These functions will play an important role in the calculation of the diffusion constant:

$$M_{L,P} = \sum_{k=0}^{\infty} a^k \binom{L+1}{P+k+1} \tag{14}$$

$$N_{L,P} = \sum_{k=0}^{\infty} b^k \binom{L+1}{P-k} \tag{15}$$

$$X_{L,P} = \frac{1}{1-\alpha-\beta}\left(M_{L-1,P-1} + \frac{1-\beta}{\beta}N_{L-1,P-1}\right). \tag{16}$$

Inserting these definitions in equation (12), we obtain

$$Z_{L,P} = \frac{1-\alpha-\beta}{\alpha\beta}\left(\alpha\beta\binom{L}{P}X_{L,P} + M_{L-1,P}N_{L-1,P-1}\right) \tag{17}$$

where we have used the identity proved in [30]:

$$\sum_{x',x=1}^{\infty} a^{x'-1}b^{x-1}\binom{L}{P+x'-x} = -\alpha\beta X_{L,P}. \tag{18}$$

Using the first equality of equation (A2), we eliminate the binomial coefficient from equation (17) and obtain

$$
\begin{aligned}
Z_{L,P} &= \frac{1-\alpha-\beta}{\alpha\beta}\left(\alpha\beta\left(N_{L,P}-\frac{N_{L-1,P-1}}{\beta}\right)X_{L,P}+M_{L-1,P}N_{L-1,P-1}\right)\\
&= \frac{1-\alpha-\beta}{\alpha\beta}(N_{L-1,P-1}(M_{L-1,P}-\alpha X_{L,P})+\alpha\beta N_{L,P}X_{L,P})\\
&= (1-\alpha-\beta)(N_{L,P}X_{L,P}-N_{L-1,P-1}X_{L+1,P+1}).
\end{aligned}
\tag{19}
$$

The last equality was obtained from equation (A4). Now expressing the function $X_{L,P}$ in terms of $M_{L,P}$ and $N_{L,P}$ (see equation (A3)), and using the Pascal triangle relations, we obtain the following identities for $Z_{L,P}$:

$$
\begin{aligned}
Z_{L,P} &= M_{L-1,P-1}N_{L,P} - M_{L,P}N_{L-1,P-1}\\
Z_{L,P} &= M_{L,P}N_{L-1,P} - M_{L-1,P}N_{L,P}\\
Z_{L,P} &= M_{L-1,P-1}N_{L-1,P} - M_{L-1,P}N_{L-1,P-1}.
\end{aligned}
\tag{20}
$$

Using these identities in equation (8), we obtain an alternative expression for v:

$$
\begin{aligned}
v &= \frac{(N_{L-1,P}M_{L-2,P-1}-M_{L-1,P}N_{L-2,P-1})-(M_{L-1,P-1}N_{L-2,P-1}-M_{L-2,P-1}N_{L-1,P-1})}{Z_{L,P}}\\
&= \frac{N_{L,P}M_{L-2,P-1}-M_{L,P}N_{L-2,P-1}}{Z_{L,P}}.
\end{aligned}
\tag{21}
$$

The derivatives of $M_{L,P}$ and $N_{L,P}$ will also be necessary for our calculations:

$$
\tilde{M}_{L,P} = \frac{\mathrm{d}M_{L,P}}{\mathrm{d}a} = \sum_{k=0}^{\infty}(k+1)a^k\binom{L+1}{P+k+2} \tag{22}
$$

$$
\tilde{N}_{L,P} = \frac{\mathrm{d}N_{L,P}}{\mathrm{d}b} = \sum_{k=0}^{\infty}(k+1)b^k\binom{L+1}{P-k-1}. \tag{23}
$$

The functions $M_{L,P}$, $N_{L,P}$, $X_{L,P}$, $\tilde{M}_{L,P}$ and $\tilde{N}_{L,P}$ satisfy many remarkable combinatorial identities and particularly the Pascal triangle recursion (i.e. $M_{L,P} = M_{L-1,P} + M_{L-1,P-1}$). Other useful identities are given in appendix A.

2.4. Generalized stationary weights

The diffusion constant of the impurity will be calculated following the method explained in [31, 33]. Let Y_t be the random variable representing the total distance travelled by the impurity between times 0 and t. The long time behaviour of $\langle Y_t|\mathcal{C}\rangle$, the average of Y_t over all histories starting with the initial configuration $\mathcal{C}$, is given by [33]

$$
\langle Y_t|\mathcal{C}\rangle \to vt + s(\mathcal{C}). \tag{24}
$$

The memory of the initial configuration is kept in the subdominant term $s(\mathcal{C})$ that provides a set of generalized weights associated with each configuration and which are related to unequal time correlation functions (see section 5.3). We shall denote the average of Y_t in the stationary state by $\langle Y_t\rangle$,

$$
\langle Y_t\rangle = \sum_{\mathcal{C}}\langle Y_t|\mathcal{C}\rangle p(\mathcal{C}). \tag{25}
$$

From the asymptotic behaviour (24), we deduce

$$
\langle Y_t|\mathcal{C}\rangle - \langle Y_t\rangle \to s(\mathcal{C}) - \sum_{\mathcal{C}} s(\mathcal{C})p(\mathcal{C}). \tag{26}
$$

In order to derive the linear equations satisfied by the generalized weights $s(\mathcal{C})$, we start with the backward master equation for the joint probability $P_t(Y, \mathcal{C}|\mathcal{C}_0)$,

$$\frac{\mathrm{d}}{\mathrm{d}t} P_t(Y, \mathcal{C}|\mathcal{C}_0) = \sum_{\mathcal{C}_1} P_t(Y, \mathcal{C}|\mathcal{C}_1)\mathcal{M}_0(\mathcal{C}_1, \mathcal{C}_0) + P_t(Y-1, \mathcal{C}|\mathcal{C}_1)\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) + P_t(Y+1, \mathcal{C}|\mathcal{C}_1)\mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0) \tag{27}$$

where $\mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0)$, $\mathcal{M}_0(\mathcal{C}_1, \mathcal{C}_0)$ and $\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0)$ are rates for transitions from $\mathcal{C}_0$ to $\mathcal{C}_1$ in which the impurity is overtaken by a normal particle does not move or hops forward.

The equation for the time evolution of the average $\langle Y_t|\mathcal{C}\rangle$ follows from (27). Inserting the asymptotic behaviour (24) in equation (27) leads to the master equation for the generalized weights,

$$\sum_{\mathcal{C}_1} s(\mathcal{C}_1)\mathcal{M}(\mathcal{C}_1, \mathcal{C}_0) = v - \sum_{\mathcal{C}_1} (\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) - \mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0)) \tag{28}$$

where

$$v = \sum_{\mathcal{C}_1, \mathcal{C}_0} p(\mathcal{C}_0)(\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) - \mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0)). \tag{29}$$

Hence, the generalized weights $s(\mathcal{C})$ can be calculated by solving a linear system of inhomogeneous equations. We note that the left-hand side of equation (28) is dual to the left-hand side of equation (3). The weights $s(\mathcal{C})$ are uniquely defined by the system (28) except for an additive constant that corresponds to a change in the origin of time in equation (24).

2.5. *Formal expression of the diffusion constant*

Time evolution of the variance of Y_t is deduced from equation (27):

$$\frac{\mathrm{d}\left(\left\langle Y_t^2\right\rangle - \langle Y_t\rangle^2\right)}{\mathrm{d}t} = 2\sum_{\mathcal{C}_0, \mathcal{C}_1} p(\mathcal{C}_0)(\langle Y_t|\mathcal{C}_1\rangle - \langle Y_t\rangle)(\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) - \mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0)) + \sum_{\mathcal{C}_0, \mathcal{C}_1} p(\mathcal{C}_0)(\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) + \mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0)). \tag{30}$$

Substituting the asymptotic behaviour (26) in equation (30) and using equation (29), we deduce that in the long time limit the variance of Y_t grows linearly with time, i.e. $\left\langle Y_t^2\right\rangle - \langle Y_t\rangle^2 \to \Delta t$ where the diffusion constant Δ is given by

$$\Delta = \sum_{\mathcal{C}_0, \mathcal{C}_1} p(\mathcal{C}_0)(\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) + \mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0)) + 2\sum_{\mathcal{C}_0, \mathcal{C}_1} s(\mathcal{C}_1)(\mathcal{M}_1(\mathcal{C}_1, \mathcal{C}_0) - \mathcal{M}_{-1}(\mathcal{C}_1, \mathcal{C}_0))p(\mathcal{C}_0) - 2v\sum_{\mathcal{C}_1} s(\mathcal{C}_1)p(\mathcal{C}_1). \tag{31}$$

Introducing *bra* and *ket* notations for the vectors $s(\mathcal{C})$ and $p(\mathcal{C})$, respectively, and defining $\langle 0| = (1, 1, \ldots, 1)$, we rewrite equation (31) in a more compact form,

$$\Delta = \langle 0|\mathcal{M}_1 + \mathcal{M}_{-1}|\mathcal{P}\rangle + 2\langle \mathcal{S}|\mathcal{M}_1 - \mathcal{M}_{-1}|\mathcal{P}\rangle - 2v\langle \mathcal{S}|\mathcal{P}\rangle. \tag{32}$$

3. Quadratic algebra for the generalized stationary weights

In this section, we solve the system of equations (28) by expressing $s(\mathcal{C})$ as a trace of a product of matrices belonging to a suitably chosen quadratic algebra.

3.1. Matrix equations

Because equations (28) defining the generalized weights are dual to those for the stationary probabilities (3), we represent the particles by the operator E and holes by the operator D. The operators D and E have been defined in equations (5) and (6). The impurity will be represented by a matrix B to be determined. We emphasize again that the ansatz for the $s(\mathcal{C})$ is *dual* to the usual one (the roles of D and E have been interchanged); *here, D stands for a hole and E for a particle*. After substituting this ansatz in (28), we find the matrix equations that B must satisfy,

$$\begin{aligned}
&\mathrm{Tr}((DB + BE - DBE)W_{L-2,P-1}) = v\\
&\mathrm{Tr}((\alpha D^2 B - \alpha DBD + BD - DB)W_{L-2,P}) = v - \alpha\\
&\mathrm{Tr}((\beta BE^2 - \beta EBE + EB - BE)W_{L-2,P-2}) = v + \beta\\
&\mathrm{Tr}((\alpha EDB + \beta BED - EB - BD + (1-\alpha-\beta)EBD)W_{L-2,P-1}) = v - \alpha + \beta
\end{aligned} \tag{33}$$

where the operator $W_{L,P}$ represents a configuration of size L with P particles (i.e. P matrices E) and $L - P$ holes (i.e. $L - P$ matrices D). A remarkable fact is that the right-hand sides in equations (33) depend only on the total number of D and E in the configuration represented by the operator $W_{L,P}$, but not on the order of the matrices D and E in $W_{L,P}$.

3.2. A new diffusion algebra

We solve the homogeneous system associated with equations (33) by introducing a suitable quadratic algebra. This algebra is a particular case of the general diffusion algebras studied in [18]. Let us consider two matrices M and N that satisfy the following identities,

$$DM = \frac{1}{\alpha}M + D \qquad ME = EM = \frac{1}{1-\alpha}M - \frac{\alpha}{1-\alpha}E \tag{34}$$

and

$$ND = DN = \frac{1}{1-\beta}N - \frac{\beta}{1-\beta}D \qquad NE = \frac{1}{\beta}N + E. \tag{35}$$

The operators M and N can be expressed as functions of E and D, respectively, as follows:

$$M = \alpha\sum_{k=0}^{\infty}(1-\alpha)^k E^{k+1} = 1 + \frac{1}{\alpha}\epsilon\sum_{k=0}^{\infty}\left(\frac{1-\alpha}{\alpha}\right)^k \epsilon^k \qquad \text{where} \quad \epsilon = E - 1 \tag{36}$$

$$N = \beta\sum_{k=0}^{\infty}(1-\beta)^k D^{k+1} = 1 + \frac{1}{\beta}\delta\sum_{k=0}^{\infty}\left(\frac{1-\beta}{\beta}\right)^k \delta^k \qquad \text{where} \quad \delta = D - 1. \tag{37}$$

Using relations (34), we verify that M satisfies the homogeneous matrix equations associated with (33), i.e. we have

$$\begin{aligned}
&DM + ME - DME = 0\\
&\alpha D^2 M - \alpha DMD + MD - DM = 0\\
&\beta ME^2 - \beta EME + EM - ME = 0\\
&\alpha EDM + \beta MED - EM - MD + (1-\alpha-\beta)EMD = 0.
\end{aligned} \tag{38}$$

The operator N also satisfies these equations and therefore any linear combination $c_m M + c_n N$ is also a solution of equations (38).

3.3. Matrix ansatz

In the algebra (M, N, D, E), traces are not well defined, e.g. $\mathrm{Tr}(MDE) = \infty$. In this section, we shall define a linear functional that extends the usual trace operation and leads to finite results. With this generalized trace, we shall obtain a matrix ansatz for the generalized weights $s(\mathcal{C})$.

There are two equivalent ways to achieve this goal. Both rely on the following property of the matrices D and E: if W_1 and W_2 are two monomials of the same degree in D and E (i.e. they contain the same number of D and the same number of E) then $W_1 - W_2$ is a finite-rank matrix. This property follows by recursion from the fact that the commutator $[D, E]$ is a matrix of finite rank. Thus, even if the traces are not well defined in the (D, E) algebra, the difference between the traces of two operators of the same degree in D and E is a finite number.

In order to regularize the traces in the (M, N, D, E) algebra, one can use a cut-off procedure as done in [31]: before calculating the trace of an operator, multiply it by the finite-rank projector $\mathbf{1}_\Lambda = \sum_{i\leqslant\Lambda} |i\rangle\langle i|$ with $\Lambda > L$. This method allows us to define a matrix ansatz but has the drawback of introducing a size-dependent parameter Λ that makes the calculations cumbersome.

We prefer to use here an analytic size-independent regularization. We first introduce a regularization matrix $\mathcal{N}$, function of a parameter t such that $|t| < 1$,

$$\mathcal{N} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & t & 0 & 0 & \cdots \\ 0 & 0 & t^2 & 0 & \cdots \\ 0 & 0 & 0 & t^3 & \cdots \\ \vdots & \vdots & \vdots & \cdots & \cdots \end{pmatrix}. \tag{39}$$

Consider now an operator $W_{L,P}$ obtained from the product of P matrices E and $L - P$ matrices D. The following properties are true,

$$\mathrm{Tr}(\mathcal{N} M W_{L,P}) = \frac{M_{L,P}}{1-t} + l_M(t; W_{L,P}) \tag{40}$$

$$\mathrm{Tr}(\mathcal{N} N W_{L,P}) = \frac{N_{L,P}}{1-t} + l_N(t; W_{L,P}) \tag{41}$$

where $l_M(t; W_{L,P})$ and $l_N(t; W_{L,P})$ are finite at $t = 1$; the functions $M_{L,P}$ and $N_{L,P}$ were defined in equations (14) and (15). The proof of equations (40) and (41) results from the fact that if W_1 and W_2 are two operators, each being a product of P matrices E and $L - P$ matrices D taken in different orders, then $\mathrm{Tr}(\mathcal{N} N(W_1 - W_2))$ has a finite limit when $t \to 1$ because, as explained above, $(W_1 - W_2)$ is a finite-rank matrix. Therefore the singularity of $\mathrm{Tr}(\mathcal{N} M W_{L,P})$ (and that of $\mathrm{Tr}(\mathcal{N} N W_{L,P})$) at $t = 1$ is independent of $W_{L,P}$ and can be calculated explicitly by taking $W_{L,P} = D^{L-P} E^P$.

If we now choose B to be

$$B = c_m M + c_n N \qquad \text{with} \quad c_m = \frac{N_{L,P}}{Z_{L,P}} \quad \text{and} \quad c_n = -\frac{M_{L,P}}{Z_{L,P}} \tag{42}$$

and take a linear combination of equations (40) and (41), we obtain

$$\mathrm{Tr}(\mathcal{N} B W_{L,P}) = \frac{c_m M_{L,P} + c_n N_{L,P}}{1-t} + l_B(t; W_{L,P}) = l_B(t; W_{L,P}) \tag{43}$$

where $l_B = c_m l_M + c_n l_N$ is finite at $t = 1$. We have thus defined a regularized trace operation and we shall write

$$\mathrm{Tr}(B W_{L,P}) = \lim_{t\to 1} \mathrm{Tr}(\mathcal{N} B W_{L,P}). \tag{44}$$

The trace operation so defined is a linear functional on the matrix algebra (M, N, D, E). However, we emphasize that this trace is not cyclic anymore. The matrix ansatz for the generalized weights $s(\mathcal{C})$ is given by

$$s(\mathcal{C}) = \mathrm{Tr}\left(B\prod_{i=1}^{L}(\tau_i(\mathcal{C})E + (1-\tau_i(\mathcal{C}))D)\right) \tag{45}$$

where B is given by equation (42) and $\tau_i(\mathcal{C}) = 0$ or 1 according to whether site i is empty or occupied by a particle in the configuration $\mathcal{C}$. In order to prove this matrix ansatz, we must verify that the generalized weights $s(\mathcal{C})$ defined in equation (45) satisfy equations (33). In the first equation, we have to evaluate $\mathrm{Tr}((D\mathcal{N}B + \mathcal{N}BE - D\mathcal{N}BE)W_{L-2,P-1})$. Using the following identity,

$$[D, \mathcal{N}] = (1-t)\mathcal{N}(1-D) \tag{46}$$

and the fact that B is a solution of the homogeneous equations (38) we deduce that

$$\begin{aligned}
&\mathrm{Tr}((D\mathcal{N}B + \mathcal{N}BE - D\mathcal{N}BE)W_{L-2,P-1})\\
&\quad = \mathrm{Tr}(([D,\mathcal{N}](B - BE) + \mathcal{N}(DB + BE - DBE))W_{L-2,P-1})\\
&\quad = (1-t)\mathrm{Tr}(\mathcal{N}(1-D)B(1-E)W_{L-2,P-1})\\
&\quad = (1-t)\left(\frac{c_m M_{L-2,P-1} + c_n N_{L-2,P-1}}{1-t} + \text{finite terms at } t=1\right).
\end{aligned} \tag{47}$$

In the $t \to 1$ limit, equation (47) reduces to

$$\frac{N_{L,P}M_{L-2,P-1} - M_{L,P}N_{L-2,P-1}}{Z_{L,P}} = v. \tag{48}$$

The last equality follows from equation (21). The proof of the other three equations of the system (33) is similar and will not be given here.

3.4. The diffusion constant as a trace

We can now express the diffusion constant Δ as a sum of traces in the tensor product algebra of the two quadratic algebras (A, D, E) and (B, E, D). Let $\mathcal{G}_{L,P}$ denote the sum of all the matrix products on this tensor algebra containing P matrices $D \otimes E$, and $L - P$ matrices $E \otimes D$. Using the two matrix ansatze (4) and (45), we obtain the following expressions:

$$\begin{aligned}
\langle\mathcal{S}|\mathcal{P}\rangle &= \frac{1}{Z_{L,P}}\mathrm{Tr}((A\otimes B)\mathcal{G}_{L,P})\\
\langle\mathcal{S}|\mathcal{M}_1|\mathcal{P}\rangle &= \frac{1}{Z_{L,P}}\mathrm{Tr}((A\otimes DB)\mathcal{G}_{L-1,P})\\
\langle\mathcal{S}|\mathcal{M}_{-1}|\mathcal{P}\rangle &= \frac{1}{Z_{L,P}}\mathrm{Tr}((A\otimes BE)\mathcal{G}_{L-1,P-1}).
\end{aligned} \tag{49}$$

Substituting equations (42) and (49) in equation (32), we obtain an expression for the diffusion constant in terms of the regularized matrix traces:

$$\begin{aligned}
\Delta = {} & \frac{Z_{L-1,P} + Z_{L-1,P-1}}{Z_{L,P}}\\
& + \frac{2c_n}{Z_{L,P}}(-v\,\mathrm{Tr}[(A\otimes N)\mathcal{G}_{L,P}] + \mathrm{Tr}[(A\otimes DN)\mathcal{G}_{L-1,P}]\\
& - \mathrm{Tr}[(A\otimes NE)\mathcal{G}_{L-1,P-1}])\\
& + \frac{2c_m}{Z_{L,P}}(-v\mathrm{Tr}[(A\otimes M)\mathcal{G}_{L,P}] + \mathrm{Tr}[(A\otimes DM)\mathcal{G}_{L-1,P}]\\
& - \mathrm{Tr}[(A\otimes ME)\mathcal{G}_{L-1,P-1}]).
\end{aligned} \tag{50}$$

Thus, to calculate Δ, we have to evaluate the six traces appearing in equation (50).

4. Calculation of the diffusion constant

4.1. Matrix elements of $\mathcal{G}_{L,P}$

The key ingredients to calculate the traces in equation (50) are the matrix elements of the 'propagator' $\mathcal{G}_{L,P}$. These matrix elements will be found by interpreting $\mathcal{G}_{L,P}$ as a random walk generator. The identity

$$\mathcal{G}_{L,P} = \mathcal{G}_{L-1,P}(E \otimes D) + \mathcal{G}_{L-1,P-1}(D \otimes E) \tag{51}$$

leads to the following recursion relation between matrix elements,

$$\begin{aligned}\langle y'|\langle x'|\mathcal{G}_{L,P}|x\rangle|y\rangle = {} & \langle y'|\langle x'|\mathcal{G}_{L-1,P}|x\rangle|y-1\rangle + \langle y'|\langle x'|\mathcal{G}_{L-1,P}|x\rangle|y\rangle \\ & + \langle y'|\langle x'|\mathcal{G}_{L-1,P}|x+1\rangle|y-1\rangle + \langle y'|\langle x'|\mathcal{G}_{L-1,P}|x+1\rangle|y\rangle \\ & + \langle y'|\langle x'|\mathcal{G}_{L-1,P-1}|x-1\rangle|y\rangle + \langle y'|\langle x'|\mathcal{G}_{L-1,P-1}|x-1\rangle|y+1\rangle \\ & + \langle y'|\langle x'|\mathcal{G}_{L-1,P-1}|x\rangle|y\rangle + \langle y'|\langle x'|\mathcal{G}_{L-1,P-1}|x\rangle|y+1\rangle \end{aligned} \tag{52}$$

for all $x, x', y, y' \geqslant 1$ with the boundary condition that a matrix element of $\mathcal{G}_{L,P}$ vanishes whenever at least one of the variables x, x', y or y' is equal to 0. The recursion relation (52) in the total space with no boundary condition can be solved by Fourier transform and is satisfied by the following expression:

$$\binom{L}{P}\binom{L}{P+y-y'}\binom{L}{P-x+x'}. \tag{53}$$

In order to satisfy the boundary condition that $\langle y'|\langle x'|\mathcal{G}_{L,P}|x\rangle|y\rangle$ vanishes when x, x', y or $y' = 0$, expression (53) is antisymmetrized using the image method as was done to derive equation (11) and we obtain

$$\begin{aligned}\langle y'|\langle x'|\mathcal{G}_{L,P}|x\rangle|y\rangle = {} & \binom{L}{P}\binom{L}{P+y-y'}\binom{L}{P-x+x'} - \binom{L}{P-x}\binom{L}{P+y-y'}\binom{L}{P+x'} \\ & + \binom{L}{P+y+x'}\binom{L}{P-y'}\binom{L}{P-x} - \binom{L}{P-x+x'}\binom{L}{P+y}\binom{L}{P-y'} \\ & + \binom{L}{P-y'-x}\binom{L}{P+y}\binom{L}{P+x'} - \binom{L}{P+y+x'}\binom{L}{P-y'-x}\binom{L}{P}. \end{aligned} \tag{54}$$

4.2. Formula for the diffusion constant

We first explain how the traces appearing in formula (50) are calculated. In order to obtain $\mathrm{Tr}[(A \otimes N)\mathcal{G}_{L,P}]$, we start by evaluating $\mathrm{Tr}[(A \otimes \mathcal{N}N)\mathcal{G}_{L,P}]$:

$$\begin{aligned}&\frac{1}{\kappa^2}\mathrm{Tr}[(A \otimes \mathcal{N}N)\mathcal{G}_{L,P}] \\ &\quad = \sum_{y,x,x'} t^{y-1}a^{x'-1}b^{x-1}\left\{\langle y|\langle x'|\mathcal{G}_{L,P}|x\rangle|y\rangle + \frac{1}{\beta}\sum_{k=0}^{\infty} b^k \langle y+k+1|\langle x'|\mathcal{G}_{L,P}|x\rangle|y\rangle\right\}.\end{aligned} \tag{55}$$

We shall substitute on the right-hand side of this equation the matrix element of $\mathcal{G}_{L,P}$ (equation (54)) which consists of six terms; we shall do it in a few steps. Substituting the first two terms of equation (54) in equation (55), we obtain

$$\sum_{y,x,x'} t^{y-1} a^{x'-1} b^{x-1} \left\{ \binom{L}{P} \binom{L}{P-x+x'} - \binom{L}{P-x} \binom{L}{P+x'} \right\} \times \left\{ \binom{L}{P} + \frac{1}{\beta} \sum_{k=0}^{\infty} b^k \binom{L}{P-k-1} \right\} = \frac{1}{1-t} \frac{Z_{L,P}}{\kappa^2} N_{L,P} \tag{56}$$

where we have used equation (12) and the first equality of equation (A2). We now remark that the substitution of the four remaining terms of equation (54) in the right-hand side of equation (55) generates sums with a finite number of terms because the binomial coefficients vanish as soon as x, x', y or k are greater than L. Therefore the $t \to 1$ limit is readily obtained by taking $t = 1$ directly. We now evaluate the contribution of each of these four terms one by one. Substituting the third term of equation (54) in equation (55) leads to

$$\sum_{y,x,x'} a^{x'-1} b^{x-1} \binom{L}{P+y+x'} \binom{L}{P-x} \left\{ \binom{L}{P-y} + \frac{1}{\beta} \sum_{k=0}^{\infty} b^k \binom{L}{P-y-k-1} \right\} = N_{L-1,P-1} \sum_{y=1}^{\infty} M_{L-1,P+y} N_{L,P-y} \tag{57}$$

where we have used equations (A1) and (A2). The substitution of the fourth term leads to

$$-\sum_{y,x,x'} a^{x'-1} b^{x-1} \binom{L}{P-x+x'} \binom{L}{P+y} \left\{ \binom{L}{P-y} + \frac{1}{\beta} \sum_{k=0}^{\infty} b^k \binom{L}{P-y-k-1} \right\} = \alpha\beta X_{L,P} \sum_{y=1}^{\infty} \binom{L}{P+y} N_{L,P-y} \tag{58}$$

where we have used equations (18) and (A2). Substituting the fifth term, we obtain

$$\sum_{y,x,x'} a^{x'-1} b^{x-1} \binom{L}{P+y} \binom{L}{P+x'} \left\{ \binom{L}{P-y-x} + \frac{1}{\beta} \sum_{k=0}^{\infty} b^k \binom{L}{P-y-x-k-1} \right\} = \sum_{y=1}^{\infty} M_{L-1,P} \binom{L}{P+y} \sum_{x=1}^{\infty} b^{x-1} N_{L,P-y-x} = M_{L-1,P} \sum_{y=1}^{\infty} \tilde{N}_{L,P-y} \binom{L}{P+y} \tag{59}$$

where we have used equation (A2) to evaluate the term in braces and equation (A8) to derive the last equality. Finally, the contribution of the last term of equation (54) is

$$-\sum_{y,x,x'} a^{x'-1} b^{x-1} \binom{L}{P} \binom{L}{P+y+x'} \left\{ \binom{L}{P-y-x} + \frac{1}{\beta} \sum_{k=0}^{\infty} b^k \binom{L}{P-y-x-k-1} \right\} = -\binom{L}{P} \sum_{y=1}^{\infty} M_{L-1,P+y} \tilde{N}_{L,P-y} \tag{60}$$

where we have again used equations (A2) and (A8).

From equations (55) to (60), we conclude that

$$\frac{1}{\kappa^2}\mathrm{Tr}[(A\otimes\mathcal{N}N)\mathcal{G}_{L,P}]$$
$$= \frac{Z_{L,P}N_{L,P}}{\kappa^2(1-t)} + \sum_{y=1}^{\infty}\left(N_{L-1,P-1}M_{L-1,P+y} + \alpha\beta X_{L,P}\binom{L}{P+y}\right)N_{L,P-y}$$
$$+ \sum_{y=1}^{\infty}\left(M_{L-1,P}\binom{L}{P+y} - \binom{L}{P}M_{L-1,P+y}\right)\tilde{N}_{L,P-y}. \qquad (61)$$

We now simplify the nonsingular part of this expression. The first sum on the rhs of equation (61) is transformed with the help of the identity (see equation (A1))

$$\binom{L}{P+y} = M_{L,P+y} - \frac{1}{\alpha}M_{L-1,P+y} \qquad (62)$$

and we obtain

$$N_{L-1,P-1}M_{L-1,P+y} + \alpha\beta X_{L,P}\binom{L}{P+y}$$
$$= \alpha\beta X_{L,P}M_{L,P+y} - (\beta X_{L,P} - N_{L-1,P-1})M_{L-1,P+y}$$
$$= \alpha\beta(X_{L,P}M_{L,P+y} - X_{L+1,P}M_{L-1,P+y}) \qquad (63)$$

where the last equality follows from equation (A5). Similarly, using equation (A1) again, the second sum on the rhs of equation (61) is written as

$$M_{L-1,P}\binom{L}{P+y} - \binom{L}{P}M_{L-1,P+y} = M_{L-1,P}M_{L,P+y} - M_{L,P}M_{L-1,P+y}. \qquad (64)$$

Thus, from equations (63) and (64) we obtain a simplified form of equation (61),

$$\frac{1}{\kappa^2}\mathrm{Tr}[(A\otimes\mathcal{N}N)\mathcal{G}_{L,P}] = \frac{Z_{L,P}N_{L,P}}{\kappa^2(1-t)} + \sum_{y}\alpha\beta(X_{L,P}M_{L,P+y} - X_{L+1,P}M_{L-1,P+y})N_{L,P-y}$$
$$+ (M_{L-1,P}M_{L,P+y} - M_{L,P}M_{L-1,P+y})\tilde{N}_{L,P-y}$$
$$= \frac{Z_{L,P}N_{L,P}}{\kappa^2(1-t)} + \alpha\beta\sum_{y=1}^{\infty}(X_{L,P}M_{L,P+y} - X_{L+1,P}M_{L-1,P+y})\tilde{N}_{L,P-y+1}$$
$$- (X_{L,P+1}M_{L,P+y} - X_{L+1,P+1}M_{L-1,P+y})\tilde{N}_{L,P-y} \qquad (65)$$

where the last equality is derived by writing $N_{L,P-y} = \tilde{N}_{L,P-y+1} - \frac{1-\beta}{\beta}\tilde{N}_{L,P-y}$ (see equation (A8)) and using equation (A4).

The five other traces that appear in equation (50) can be evaluated in a similar way. In appendix B, we give the expressions of these traces, insert them in equation (50), and obtain

$$\Delta = \frac{M_{L,P}N_{L-2,P-1} + N_{L,P}M_{L-2,P-1}}{Z_{L,P}} + \frac{2(\alpha+\beta-1)}{Z_{L,P}^2}\sum_{y=1}^{\infty}$$
$$\times\{c_n(Z_{L,P}M_{L-2,P+y-1} - Z_{L-1,P}M_{L-1,P+y-1} - Z_{L-1,P-1}M_{L-1,P+y})$$
$$\times(X_{L+1,P}\tilde{N}_{L,P-y+1} - X_{L+1,P+1}\tilde{N}_{L,P-y})$$
$$+ c_m(Z_{L,P}N_{L-2,P-y-1} - Z_{L-1,P}N_{L-1,P-y-1} - Z_{L-1,P-1}N_{L-1,P-y})$$
$$\times(X_{L+1,P}\tilde{M}_{L,P+y} - X_{L+1,P+1}\tilde{M}_{L,P+y-1})\}. \qquad (66)$$

We must now calculate the twelve sums that appear in this equation. In appendix C, we calculate these sums, substitute them in equation (66), and derive the following simplified expression for the diffusion constant,

$$\Delta = \frac{Z_{L-1,P-1}\mathcal{W}_{2L+1,2P+1} + Z_{L-1,P}\mathcal{W}_{2L+1,2P} - Z_{L,P}\mathcal{W}_{2L,2P}}{Z_{L,P}^3} \tag{67}$$

where we have defined

$$\mathcal{W}_{L,P} = \alpha_0\mathcal{U}_{L,P} + \alpha_1\mathcal{U}_{L,P-1} + \alpha_2\mathcal{U}_{L,P-2} \tag{68}$$

with

$$\mathcal{U}_{L,P} = \left(\frac{1-\beta}{\beta}\right)^2 \tilde{N}_{L-1,P} + \tilde{M}_{L-1,P-1} - 2\alpha(1-\beta)X_{L,P} \tag{69}$$

and

$$\alpha_0 = X_{L+1,P}^2 \qquad \alpha_1 = -2X_{L+1,P}X_{L+1,P+1} \qquad \alpha_2 = X_{L+1,P+1}^2. \tag{70}$$

We thus obtain a closed formula for the diffusion constant in terms of the special functions defined in section 2.3. We shall now relate our expression for the diffusion constant to that derived from Bethe ansatz and discuss the physical properties of Δ.

5. Discussion

5.1. Two particular cases

When $\alpha = \beta = 1$, the impurity becomes a second-class particle [21, 22]. In this case, the matrix algebra used to calculate the diffusion constant is simpler as the matrices M and N are identical to E and D respectively. The functions $M_{L,P}$ and $N_{L,P}$ reduce to binomial coefficients

$$M_{L,P} = \binom{L+1}{P+1} \qquad N_{L,P} = \binom{L+1}{P} \qquad Z_{L,P} = \frac{1}{L+1}\binom{L+1}{P}\binom{L+1}{P+1} \tag{71}$$

and we obtain the following formula for the diffusion constant:

$$\Delta = \frac{1}{Z_{L,P}}\frac{1}{L(2L+1)}\frac{(2L+2)!}{(2P+2)!(2L-2P+2)!}\left((L-4)P(L-P) + L(2L+1)\right). \tag{72}$$

This expression was first presented in [35].

Another particular case is obtained when $\alpha + \beta = 1$ (or equivalently $ab = 1$). For this choice of parameters, the stationary state is uniform, i.e. all configurations have the same stationary probability [15, 30]. The ansatz for the $p(\mathcal{C})$ reduces to $A = 1, D = 1/\beta$ and $E = 1/\alpha$, whereas for the $s(\mathcal{C})$ the ansatz (45) is unchanged. Thus, we have

$$Z_{L,P} = \frac{1}{\alpha^{L-P}\beta^P}\binom{L}{P} \qquad \frac{1}{\alpha}M_{L,P} + \frac{1}{\beta}N_{L,P} = \frac{1}{\alpha^{L+1-P}\beta^P}$$

$$v = \alpha - \frac{P}{L} \qquad \frac{Z_{L-1,P} + Z_{L-1,P-1}}{Z_{L,P}} = \frac{(L-2P)\alpha + P}{L}. \tag{73}$$

Equation (50) for the diffusion constant reduces to

$$\Delta = \frac{(L-2P)\alpha + P}{L} + \frac{2}{\alpha^{L-P}\beta^P Z_{L,P}^2}\{c_n[\alpha\mathrm{Tr}(DNG_{L-1,L-1-P}) - \beta\mathrm{Tr}(NEG_{L-1,L-P})$$
$$- v\mathrm{Tr}(NG_{L,L-P})] + c_m[\alpha\mathrm{Tr}(DMG_{L-1,L-1-P})$$
$$- \beta\mathrm{Tr}(MEG_{L-1,L-P}) - v\mathrm{Tr}(MG_{L,L-P})]\} \tag{74}$$

where $G_{L,P}$ has been defined in equation (10) and its matrix elements are given in equation (11). Here, the calculation of the diffusion constant does not require the tensor product of two algebras but only one quadratic algebra. After simplifying equation (74), one is led to

$$\Delta = \frac{\alpha^{L-P}(1-\alpha)^P}{\binom{L}{P}^2}\left\{N_{L,P}M_{2L-1,2P-1} - M_{L,P}N_{2L-1,2P-1} - \frac{P}{L}(N_{L,P}M_{2L,2P} - M_{L,P}N_{2L,2P})\right\} - \frac{\alpha^{L-P}(1-\alpha)^P}{\binom{L}{P}^2}M_{L,P}N_{L,P} \times \left\{(1-\alpha)M_{L-1,P-1} - \alpha N_{L-1,P-1} - \frac{P}{L}((1-\alpha)M_{L,P} - \alpha N_{L,P})\right\}. \quad (75)$$

5.2. Relation with the Bethe ansatz

We now prove that the formula (67) for the diffusion constant agrees with that derived using the Bethe ansatz in [34]. Writing the binomial coefficient as a contour integral,

$$\binom{L}{P} = \oint_1 \frac{z^L}{(z-1)^{P+1}}\frac{dz}{2i\pi} \quad (76)$$

we find

$$M_{L,P} = \alpha \oint_{1,\frac{1}{\alpha}} \frac{z^{L+1}}{(z-1)^{P+1}(\alpha z-1)}\frac{dz}{2i\pi}$$

and

$$N_{L,P} = \beta \oint_1 \frac{z^{L+1}}{(z-1)^{P+1}(1-(1-\beta)z)}\frac{dz}{2i\pi}. \quad (77)$$

These two formulae allow us to find integral representations for $X_{L,P}$, $\tilde{M}_{L,P}$ and $\tilde{N}_{L,P}$. We deduce finally that $\mathcal{U}_{L,P}$, defined in equation (69), is given by

$$\mathcal{U}_{L,P} = \oint_{1,\frac{1}{\alpha}} \frac{z^L}{(z-1)^P(\alpha z-1)^2(1-(1-\beta)z)^2}\frac{dz}{2i\pi}. \quad (78)$$

Substituting this relation in equations (68) and (67) our expression for Δ agrees with that of [34]. We recall the behaviour of Δ in different parts of the phase diagram [34]:

- If $\rho < \beta$ and $\rho < 1-\alpha$, or if $\beta < \rho$ and $1-\alpha < \rho$, $\Delta \to \frac{\overline{\rho}(1-\overline{\rho})}{|\rho-\overline{\rho}|}$, where $\overline{\rho}$ is equal to α or $1-\beta$ respectively. In the limit of large systems, the defect has a normal diffusive behaviour. This contrasts with the subdiffusive behaviour (with exponent $\frac{1}{3}$) of a real hole or a real first-class particle in the ASEP [31].
- For $1-\alpha < \rho < \beta$, the defect is similar to a second-class particle [21] and shows a superdiffusive behaviour in the limit of large systems. A finite size scaling argument, using that Δ scales as $L^{1/2}$, shows that the corresponding diffusion exponent is $\frac{2}{3}$.
- In the shock phase, $\beta < \rho < 1-\alpha$, the shock has a normal diffusive behaviour with $\Delta \to \frac{\alpha(1-\alpha)+\beta(1-\beta)}{1-\alpha-\beta}$. This value of the diffusion constant can be understood by considering the shock as a random walker between a phase of low density β and a phase of high density $1-\alpha$.

5.3. Relation with correlation functions

Let us consider the following (time-integrated) unequal time correlation function in the steady state:

$$\psi(\mathcal{C}_0) = \int_0^\infty (\langle\eta\rangle - \langle\eta(t)|\mathcal{C}_0\rangle)\,\mathrm{d}t \qquad \text{where} \quad \eta = \alpha(1-\tau_1) - \beta\tau_L. \quad (79)$$

This quantity represents a numerical function associated with a configuration $\mathcal{C}_0$. Using the equality

$$\sum_{\mathcal{C}_0} \langle\tau_i(t)|\mathcal{C}_0\rangle p(\mathcal{C}_0) = \langle\tau_i\rangle$$

we derive

$$\sum_{\mathcal{C}_0} \psi(\mathcal{C}_0) p(\mathcal{C}_0) = 0. \quad (80)$$

Besides, we recall that for any site i,

$$\langle\tau_i(t)|\mathcal{C}_1\rangle = \sum_{\mathcal{C}} \tau_i(\mathcal{C}) P_t(\mathcal{C}|\mathcal{C}_1). \quad (81)$$

Hence, we deduce

$$\sum_{\mathcal{C}_1} \langle\tau_i(t)|\mathcal{C}_1\rangle \mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) = \sum_{\mathcal{C},\mathcal{C}_1} \tau_i(\mathcal{C}) P_t(\mathcal{C}|\mathcal{C}_1)\mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) = \sum_{\mathcal{C}} \tau_i(\mathcal{C}) \frac{\mathrm{d}P_t(\mathcal{C}|\mathcal{C}_0)}{\mathrm{d}t} \quad (82)$$

where we have used the backward form of the master equation (2). Taking the large time limit of equation (82) and recalling that sum over a column of the Markov matrix identically vanishes, we show that

$$\sum_{\mathcal{C}_1} \langle\tau_i|\mathcal{C}_1\rangle \mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) = \sum_{\mathcal{C},\mathcal{C}_1} \tau_i(\mathcal{C}) p(\mathcal{C}) \mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) = 0. \quad (83)$$

From equations (82) and (83), we deduce

$$\sum_{\mathcal{C}_1} \int_0^\infty (\langle\tau_i\rangle - \langle\tau_i(t)|\mathcal{C}_1\rangle)\,\mathrm{d}t\,\mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) = \sum_{\mathcal{C}_1} \tau_i(\mathcal{C}_1) \int_0^\infty \frac{\mathrm{d}P_t(\mathcal{C}_1|\mathcal{C}_0)}{\mathrm{d}t}$$
$$= \sum_{\mathcal{C}_1} \tau_i(\mathcal{C}_1)\left(p(\mathcal{C}_1) - \delta_{\mathcal{C}_1,\mathcal{C}_0}\right) = \langle\tau_i\rangle - \tau_i(\mathcal{C}_0). \quad (84)$$

Thus the correlation function ψ satisfies the following equation:

$$\sum_{\mathcal{C}_1} \psi(\mathcal{C}_1)\mathcal{M}(\mathcal{C}_1,\mathcal{C}_0) = \alpha\langle 1-\tau_1\rangle - \beta\langle\tau_L\rangle - \alpha(1-\tau_1(\mathcal{C}_0)) + \beta\tau_L(\mathcal{C}_0). \quad (85)$$

This equation is the same as equation (28) satisfied by the generalized weights $s(\mathcal{C})$. Thus from equations (79) and (80), we deduce the relation between generalized weights and correlation functions,

$$s(\mathcal{C}_0) - \sum_{\mathcal{C}_0} s(\mathcal{C}_0) p(\mathcal{C}_0) = \int_0^\infty (\langle\eta\rangle - \langle\eta(t)|\mathcal{C}_0\rangle)\,\mathrm{d}t. \quad (86)$$

Substituting this expression in equation (31), the diffusion constant can be expressed as a linear combination of correlation functions,

$$\Delta = \overline{J} + 2\sum_{\mathcal{C}_1} \int_0^\infty (\langle\eta\rangle - \langle\eta(t)|\mathcal{C}_1\rangle)\, f(\mathcal{C}_1)\,\mathrm{d}t \quad (87)$$

with

$$\overline{J} = \sum_{\mathcal{C}_0,\mathcal{C}_1} (\mathcal{M}_1(\mathcal{C}_1,\mathcal{C}_0) + \mathcal{M}_{-1}(\mathcal{C}_1,\mathcal{C}_0))\,p(\mathcal{C}_0)$$

and (88)

$$f(\mathcal{C}_1) = \sum_{\mathcal{C}_0} (\mathcal{M}_1(\mathcal{C}_1,\mathcal{C}_0) - \mathcal{M}_{-1}(\mathcal{C}_1,\mathcal{C}_0))\,p(\mathcal{C}_0).$$

In general, expression (87) cannot be reduced to a linear combination of two time correlation functions in the stationary state [8]. However, when $\alpha + \beta = 1$, the stationary probability is uniform and this implies that

$$f(\mathcal{C}_1) = \{\alpha(1-\tau_L(\mathcal{C}_1)) - \beta\tau_1(\mathcal{C}_1)\}\binom{L}{P}^{-1}. \qquad (89)$$

Then, equation (87) becomes

$$\Delta = \frac{(L-2P)\alpha + P}{L} + 2\int_0^\infty \left\{\left(\alpha - \frac{P}{L}\right)^2 - \langle[\alpha(1-\tau_1(t)) - \beta\tau_L(t)] \times [\alpha(1-\tau_L(0)) - \beta\tau_1(0)]\rangle\right\} \mathrm{d}t. \qquad (90)$$

6. Conclusion

In this work, we have shown that the diffusion constant of an impurity in the ASEP can be calculated by using an extension of the matrix approach. We have also obtained matrix expressions for a set of unequal time correlation functions. Hence, for the ASEP, the matrix method is a versatile tool that allows us to calculate stationary state properties as well as non-stationary properties. One advantage of the matrix technique is that it provides closed expressions for properties of a given configuration and not for global quantities only, e.g. the stationary probability or the generalized weight of a configuration when expressed as a matrix element can be calculated without referring to other configurations. This contrasts with the Bethe ansatz approach, in which the eigenvalues of the Markov matrix are determined by a set of coupled nonlinear polynomial equations. Although the diffusion constant, given as a symmetric combination of these eigenvalues, can be calculated without solving explicitly these equations, the eigenvectors of the Markov matrix cannot be expressed in a simple manner; therefore, finding correlation functions from the Bethe ansatz is usually a formidable task.

The matrix ansatz and the Bethe ansatz are complementary techniques. Nevertheless, they seem to be intimately related [36, 37]. One of our goals in studying this problem was to find a system with a non-trivial stationary state where both methods apply and can be related to each other in a systematic manner. We believe that a matrix ansatz exists for any ASEP problem solved by the Bethe ansatz; in particular, it would be very interesting to understand how the matrix method can be extended to find all moments of the time-integrated current in the pure ASEP, which were calculated in [38] using the Bethe ansatz. Certainly, for calculating higher moments, multiple tensor products of quadratic algebras, analogous to those used for ASEP with multiple species [24], will be involved. The ASEP with open boundaries provides the example of an integrable system [17] for which the matrix method allows us to calculate the steady state [15] and the fluctuations of the current [33]. However, due to the lack of a reference state, it has not been possible to perform a Bethe ansatz for this system and the calculation of higher order fluctuations and of large deviation functions is still out of reach.

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Appendix A. Some useful combinatorial identities

In order to calculate the normalization factor $Z_{L,P}$ we introduced generalized binomial coefficients $M_{L,P}$, $N_{L,P}$ and $X_{L,P}$. In this appendix, we give some useful identities that are satisfied by these functions:

$$\begin{aligned} M_{L,P} &= \binom{L}{P} + \frac{1}{\alpha}\sum_{k=0}^{\infty} a^k \binom{L}{P+k+1} = \binom{L}{P} + \frac{1}{\alpha} M_{L-1,P} \\ &= \frac{1}{1-\alpha} M_{L-1,P-1} - \frac{\alpha}{1-\alpha}\binom{L}{P} = \frac{1-\alpha}{\alpha} M_{L,P+1} + \binom{L+1}{P+1} \end{aligned} \tag{A1}$$

$$\begin{aligned} N_{L,P} &= \binom{L}{P} + \frac{1}{\beta}\sum_{k=0}^{\infty} b^k \binom{L}{P-k-1} = \binom{L}{P} + \frac{1}{\beta} N_{L-1,P-1} \\ &= \frac{1}{1-\beta} N_{L-1,P} - \frac{\beta}{1-\beta}\binom{L}{P} = \frac{1-\beta}{\beta} N_{L,P-1} + \binom{L+1}{P} \end{aligned} \tag{A2}$$

$$\begin{aligned} X_{L,P} &= \frac{1}{1-\alpha-\beta}\left(M_{L-1,P-1} + \frac{1-\beta}{\beta} N_{L-1,P-1}\right) \\ &= \frac{1}{1-\alpha-\beta}\left(\frac{1-\alpha}{\alpha} M_{L-1,P} + N_{L-1,P}\right) \\ &= \frac{1}{1-\alpha-\beta}\left(\frac{1}{\alpha} M_{L-2,P-1} + \frac{1}{\beta} N_{L-2,P-1}\right) \end{aligned} \tag{A3}$$

$$M_{L,P} = \alpha\beta\left(\frac{1-\beta}{\beta} X_{L+1,P} - X_{L+1,P+1}\right) = \alpha X_{L+1,P} - \alpha\beta X_{L+2,P+1} \tag{A4}$$

$$N_{L,P} = \alpha\beta\left(\frac{1-\alpha}{\alpha} X_{L+1,P+1} - X_{L+1,P}\right) = \beta X_{L+1,P+1} - \alpha\beta X_{L+2,P+1}. \tag{A5}$$

If we eliminate $N_{L,P}$ from equation (19) by using equation (A5), we obtain

$$\begin{aligned} Z_{L,P} &= \alpha\beta(1-\alpha-\beta)(X_{L+1,P+1}X_{L,P-1} - X_{L+1,P}X_{L,P}) \\ &= \alpha\beta(1-\alpha-\beta)\left(X_{L+2,P+1}X_{L,P-1} - X_{L+1,P}^2\right) \\ &= \alpha\beta(1-\alpha-\beta)(X_{L+1,P}X_{L,P+1} - X_{L+1,P+1}X_{L,P}) \\ &= \alpha\beta(1-\alpha-\beta)\left(X_{L+2,P+1}X_{L,P+1} - X_{L+1,P+1}^2\right) \end{aligned} \tag{A6}$$

other equivalent identities can be derived using the Pascal triangle relations for $X_{L,P}$. We shall also need the following relations:

$$\begin{aligned} \tilde{M}_{L,P} &= \sum_{k=1}^{\infty} a^{k-1} M_{L,P+k} = M_{L-1,P} + \frac{1}{\alpha}\tilde{M}_{L-1,P} \\ &= \frac{1}{1-\alpha}\tilde{M}_{L-1,P-1} - \frac{\alpha}{1-\alpha} M_{L-1,P} = \frac{1-\alpha}{\alpha}\tilde{M}_{L,P+1} + M_{L,P+1} \end{aligned} \tag{A7}$$

$$\tilde{N}_{L,P} = \sum_{k=1}^{\infty} b^{k-1} N_{L,P-k} = N_{L-1,P-1} + \frac{1}{\beta}\tilde{N}_{L-1,P-1}$$
$$= \frac{1}{1-\beta}\tilde{N}_{L-1,P} - \frac{\beta}{1-\beta}N_{L-1,P-1} = \frac{1-\beta}{\beta}\tilde{N}_{L,P-1} + N_{L,P-1}. \tag{A8}$$

We also have the following relations between $X_{L,P}$ and $Z_{L,P}$:

$$Z_{L-1,P}X_{L,P} + Z_{L-1,P-1}X_{L,P+1} = Z_{L,P}X_{L-1,P} \tag{A9}$$

$$Z_{L-1,P}X_{L,P-1} + Z_{L-1,P-1}X_{L,P} = Z_{L,P}X_{L-1,P-1}. \tag{A10}$$

These relations lead to

$$vX_{L,P} - X_{L-1,P} = -\frac{Z_{L-1,P-1}}{Z_{L,P}}X_{L+1,P+1} \tag{A11}$$

$$vX_{L,P} + X_{L-1,P-1} = \frac{Z_{L-1,P}}{Z_{L,P}}X_{L+1,P} \tag{A12}$$

$$vX_{L,P-1} - X_{L-1,P-1} = -\frac{Z_{L-1,P-1}}{Z_{L,P}}X_{L+1,P} \tag{A13}$$

$$vX_{L,P+1} + X_{L-1,P} = \frac{Z_{L-1,P}}{Z_{L,P}}X_{L+1,P+1}. \tag{A14}$$

Appendix B. Expressions of the traces and derivation of equation (66)

In this appendix, we give the expressions of the traces that appear in formula (50) and we derive equation (66). All the traces can be calculated in a way similar to that explained in section 4.2. We only give the results here and as in section 4.2 we write the singular term when $t \to 1$ and the principal value of the trace at $t = 1$. Thus we have

$$\frac{1}{\kappa^2}\operatorname{Tr}[(A \otimes D\mathcal{N}N)\mathcal{G}_{L-1,P}]$$
$$= \frac{1}{\kappa^2}\operatorname{Tr}[(A \otimes [D,\mathcal{N}]N)\mathcal{G}_{L-1,P}] + \frac{1}{\kappa^2}\operatorname{Tr}[(A \otimes \mathcal{N}DN)\mathcal{G}_{L-1,P}]$$
$$= \frac{Z_{L-1,P}N_{L,P}}{\kappa^2(1-t)} - \frac{Z_{L-1,P}N_{L-1,P-1}}{\kappa^2} + \alpha\beta\sum_{y=1}^{\infty}\{(X_{L-1,P}M_{L-1,P+y}$$
$$- X_{L,P}M_{L-2,P+y})\tilde{N}_{L,P-y+1} - (X_{L-1,P+1}M_{L-1,P+y}$$
$$- X_{L,P+1}M_{L-2,P+y})\tilde{N}_{L,P-y}\} \tag{B1}$$

$$\frac{1}{\kappa^2}\operatorname{Tr}[(A \otimes \mathcal{N}NE)\mathcal{G}_{L-1,P-1}] = \frac{Z_{L-1,P-1}N_{L,P}}{\kappa^2(1-t)} + \alpha\beta\sum_{y=1}^{\infty}\{(X_{L-1,P-1}M_{L-1,P+y-1}$$
$$- X_{L,P-1}M_{L-2,P+y-1})\tilde{N}_{L,P-y+1} - (X_{L-1,P}M_{L-1,P+y-1}$$
$$- X_{L,P}M_{L-2,P+y-1})\tilde{N}_{L,P-y}\}. \tag{B2}$$

The calculation of the other three traces that involve the M matrix is simplified if the matrix M acts on the ket, i.e. if M is on the left of $\mathcal{N}$. Thus we have

$$\begin{aligned}
&\frac{1}{\kappa^2}\,\mathrm{Tr}[(A\otimes\mathcal{N}M)\mathcal{G}_{L,P}]\\
&\qquad=\frac{1}{\kappa^2}\mathrm{Tr}[A\otimes(\mathcal{N}M-M\mathcal{N})\mathcal{G}_{L,P}]+\frac{1}{\kappa^2}\,\mathrm{Tr}[(A\otimes M\mathcal{N})\mathcal{G}_{L,P}]\\
&\qquad=\frac{Z_{L,P}M_{L,P}}{\kappa^2(1-t)}-\frac{Z_{L,P}\tilde{M}_{L-1,P-1}}{\alpha\kappa^2}+\alpha\beta\sum_{y=1}^{\infty}\{(X_{L,P}N_{L,P-y}\\
&\qquad\quad-X_{L+1,P+1}N_{L-1,P-y-1})\tilde{M}_{L,P+y-1}-(X_{L,P-1}N_{L,P-y}\\
&\qquad\quad-X_{L+1,P}N_{L-1,P-y-1})\tilde{M}_{L,P+y}\}
\end{aligned}\tag{B3}$$

$$\begin{aligned}
&\frac{1}{\kappa^2}\mathrm{Tr}[(A\otimes D\mathcal{N}M)\mathcal{G}_{L-1,P}]\\
&\qquad=\frac{1}{\kappa^2}\,\mathrm{Tr}[(A\otimes D[\mathcal{N},M])\mathcal{G}_{L-1,P}]+\frac{1}{\kappa^2}\,\mathrm{Tr}[(A\otimes DM\mathcal{N})\mathcal{G}_{L-1,P}]\\
&\qquad=\frac{Z_{L-1,P}M_{L,P}}{\kappa^2(1-t)}-\frac{Z_{L-1,P}\tilde{M}_{L-1,P-1}}{\alpha\kappa^2}+\alpha\beta\sum_{y=1}^{\infty}\{(X_{L-1,P}N_{L-1,P-y}\\
&\qquad\quad-X_{L,P+1}N_{L-2,P-y-1})\tilde{M}_{L,P+y-1}\\
&\qquad\quad-(X_{L-1,P-1}N_{L-1,P-y}-X_{L,P}N_{L-2,P-y-1})\tilde{M}_{L,P+y}\}
\end{aligned}\tag{B4}$$

$$\begin{aligned}
&\frac{1}{\kappa^2}\mathrm{Tr}[(A\otimes\mathcal{N}ME)\mathcal{G}_{L-1,P-1}]\\
&\qquad=\frac{1}{\kappa^2}\,\mathrm{Tr}[(A\otimes[\mathcal{N},ME])\mathcal{G}_{L-1,P-1}]+\frac{1}{\kappa^2}\,\mathrm{Tr}[(A\otimes ME\mathcal{N})\mathcal{G}_{L-1,P-1}]\\
&\qquad=\frac{Z_{L-1,P-1}M_{L,P}}{\kappa^2(1-t)}-\frac{Z_{L-1,P-1}\tilde{M}_{L-1,P-1}}{\alpha\kappa^2}-\frac{Z_{L-1,P-1}M_{L-1,P}}{\kappa^2}\\
&\qquad\quad+\alpha\beta\sum_{y=1}^{\infty}\{(X_{L-1,P-1}N_{L-1,P-y-1}-X_{L,P}N_{L-2,P-y-2})\tilde{M}_{L,P+y-1}\\
&\qquad\quad-(X_{L-1,P-2}N_{L-1,P-y-1}-X_{L,P-1}N_{L-2,P-y-2})\tilde{M}_{L,P+y}\}.
\end{aligned}\tag{B5}$$

In order to derive expression (66) for the diffusion constant, we insert equations (65) and (B1) to (B5) in formula (50). First, we remark that when we take the linear combination $c_n\,\mathrm{Tr}[(A\otimes\mathcal{N}N)\mathcal{G}_{L,P}]+c_m\,\mathrm{Tr}[(A\otimes\mathcal{N}M)\mathcal{G}_{L,P}]$ the singular terms appearing in equations (65) and (B3) cancel out. Similarly, all other singular terms of the type $1/(1-t)$ cancel out from formula (50).

We now consider the terms that are independent of y. The terms containing the factor $\tilde{M}_{L-1,P-1}$ cancel out: indeed inserting them in equation (50) and collecting them, we obtain

$$\frac{2c_m}{\alpha\kappa^2 Z_{L,P}}(vZ_{L,P}-Z_{L-1,P}+Z_{L-1,P-1})\tilde{M}_{L-1,P-1}.\tag{B6}$$

Using the formula (8) for the speed v, this expression is found to be equal to zero. The other y independent terms add up with the first term on the right-hand side of equation (50) and we group them together as follows:

$$\frac{Z_{L-1,P} + Z_{L-1,P-1}}{Z_{L,P}} + \frac{2}{Z_{L,P}}(c_m Z_{L-1,P-1} M_{L-1,P} - c_n Z_{L-1,P} N_{L-1,P-1})$$
$$= \frac{1}{Z_{L,P}^2}(Z_{L-1,P}(Z_{L,P} + 2M_{L,P}N_{L-1,P-1}) + Z_{L-1,P-1}(Z_{L,P} + 2M_{L-1,P}N_{L,P}))$$
$$= \frac{1}{Z_{L,P}^2}((M_{L-2,P-1}N_{L-1,P} - M_{L-1,P}N_{L-2,P-1})(M_{L-1,P-1}N_{L,P} + M_{L,P}N_{L-1,P-1}) + (M_{L-1,P-1}N_{L-2,P-1} - M_{L-2,P-1}N_{L-1,P-1})(M_{L,P}N_{L-1,P} + M_{L-1,P}N_{L,P}))$$
$$= \frac{1}{Z_{L,P}}(M_{L,P}N_{L-2,P-1} + N_{L,P}M_{L-2,P-1}). \tag{B7}$$

We have used here the formula (42) for c_m and c_n, and equations (20).

We complete the derivation of equation (66) from equation (50) by adding up the y-dependent terms. Considering first the traces that are multiplied by $2c_n/Z_{L,P}$ in equation (50), we have to evaluate the expression $\kappa^2(-v$ equation (65) + equation (B1) − equation (B2)), which is equal to (leaving aside, for ease of writing, a multiplicative factor $\alpha + \beta - 1$ and the symbol $\sum_{y=1}^{\infty}$)

$$-v(X_{L,P}M_{L,P+y} - X_{L+1,P}M_{L-1,P+y})\tilde{N}_{L,P-y+1} + v(X_{L,P+1}M_{L,P+y} - X_{L+1,P+1}M_{L-1,P+y}) \times \tilde{N}_{L,P-y} + (X_{L-1,P}M_{L-1,P+y} - X_{L,P}M_{L-2,P+y})\tilde{N}_{L,P-y+1} - (X_{L-1,P+1}M_{L-1,P+y} - X_{L,P+1}M_{L-2,P+y})\tilde{N}_{L,P-y} - (X_{L-1,P-1}M_{L-1,P+y-1} - X_{L,P-1}M_{L-2,P+y-1})\tilde{N}_{L,P-y+1} + (X_{L-1,P}M_{L-1,P+y-1} - X_{L,P}M_{L-2,P+y-1})\tilde{N}_{L,P-y}. \tag{B8}$$

Collecting the terms that have a common factor $\tilde{N}_{L,P-y+1}$ and using the Pascal recursion relation, we obtain

$$-vX_{L,P}(M_{L-1,P+y} + M_{L-1,P+y-1}) + vX_{L+1,P}M_{L-1,P+y} + X_{L-1,P}M_{L-1,P+y} - X_{L,P}(M_{L-1,P+y} - M_{L-2,P+y-1}) - X_{L-1,P-1}M_{L-1,P+y-1} + X_{L,P-1}M_{L-2,P+y-1}$$
$$= M_{L-1,P+y}(vX_{L,P-1} - X_{L-1,P-1}) - M_{L-1,P+y-1}(vX_{L,P} + X_{L-1,P-1}) + X_{L+1,P}M_{L-2,P+y-1}$$
$$= \frac{X_{L+1,P}}{Z_{L,P}}(Z_{L,P}M_{L-2,P+y-1} - Z_{L-1,P}M_{L-1,P+y-1} - Z_{L-1,P-1}M_{L-1,P+y}) \tag{B9}$$

where we have used equations (A12) and (A13) to derive the last equality. Similarly, the terms with a common factor $\tilde{N}_{L,P-y}$ in equation (B8) are equal to

$$vX_{L,P+1}(M_{L-1,P+y} + M_{L-1,P+y-1}) - vX_{L+1,P+1}M_{L-1,P+y} - X_{L-1,P+1}M_{L-1,P+y} + X_{L,P+1} \times (M_{L-1,P+y} - M_{L-2,P+y-1}) + X_{L-1,P}M_{L-1,P+y-1} - X_{L,P}M_{L-2,P+y-1}$$
$$= M_{L-1,P+y}(-vX_{L,P} + X_{L-1,P}) + M_{L-1,P+y-1}(vX_{L,P+1} + X_{L-1,P}) - X_{L+1,P+1}M_{L-2,P+y-1}$$
$$= -\frac{X_{L+1,P+1}}{Z_{L,P}}(Z_{L,P}M_{L-2,P+y-1} - Z_{L-1,P}M_{L-1,P+y-1} - Z_{L-1,P-1}M_{L-1,P+y}) \tag{B10}$$

where we have used equations (A11) and (A14) to derive the last equality. Substituting equations (B9) and (B10) in equation (B8), we obtain the expression that appears with the multiplicative factor c_n in equation (66). The expression with the multiplicative factor c_m in equation (66) is obtained from equations (50) and (B3), (B4) and (B5) following the same procedure. This completes the derivation of equation (66).

Appendix C. Proof of equation (67)

We first note that the generalized combinatorial functions defined in section 2.3 can be interpreted as power series coefficients thanks to the following identities between functions of the formal variable z:

$$\sum_{P=-\infty}^{+\infty} z^P M_{L,P} = \frac{(z+1)^{L+1}}{z-a} \tag{C1}$$

$$\sum_{P=-\infty}^{+\infty} z^P N_{L,P} = \frac{(z+1)^{L+1}}{1-bz} \tag{C2}$$

$$\sum_{P=-\infty}^{+\infty} z^P X_{L,P+1} = -\frac{1}{\alpha\beta}\frac{(z+1)^{L}}{(z-a)(1-bz)}. \tag{C3}$$

Equation (C1), for example, is obtained by using expression (14) for $M_{L,P}$ and summing explicitly the series thus obtained:

$$\sum_{P=-\infty}^{+\infty} M_{L,P} z^P = \sum_{k=0}^{\infty} \frac{a^k}{z^{k+1}} \sum_{P=-\infty}^{+\infty} \binom{L+1}{P+k+1} z^{P+k+1} = \frac{(z+1)^{L+1}}{z-a}. \tag{C4}$$

Taking the product of the series (C1) and (C2) and comparing the result with equation (C3), we deduce that

$$\sum_{k=-\infty}^{\infty} M_{L_1,P_1+k} N_{L_2,P_2-k} = -\alpha\beta X_{L_1+L_2+2,P_1+P_2+1}. \tag{C5}$$

Taking the derivative of this expression with respect to a and b respectively, we obtain

$$\sum_{k=-\infty}^{\infty} \tilde{M}_{L_1,P_1+k} N_{L_2,P_2-k} = \frac{1}{\kappa^2}(-\alpha(1-\beta) X_{L_1+L_2+2,P_1+P_2+1} + \tilde{M}_{L_1+L_2+1,P_1+P_2}) \tag{C6}$$

$$\sum_{k=-\infty}^{\infty} M_{L_1,P_1+k} \tilde{N}_{L_2,P_2-k} = \frac{1}{\kappa^2}(-\beta(1-\alpha) X_{L_1+L_2+2,P_1+P_2+1} + \tilde{N}_{L_1+L_2+1,P_1+P_2}). \tag{C7}$$

It should be noted that the summation variable y in sums that appear in expression (66) for the diffusion constant runs from 1 to ∞ and not from $-\infty$ to ∞. Therefore we must, first of all, symmetrize the sums involved in equation (66) in order to be able to evaluate them with the help of equations (C5), (C6) and (C7). Using equations (A4) and (A5), we write

$$\begin{aligned} M_{L,P+y} N_{L,P-y} = (\alpha\beta)^2 (ab X_{L+1,P+y} X_{L+1,P-y+1} - a X_{L+1,P+y+1} X_{L+1,P-y+1} \\ - b X_{L+1,P+y} X_{L+1,P-y} + X_{L+1,P+y+1} X_{L+1,P-y}). \end{aligned} \tag{C8}$$

Thanks to this decomposition, the sum $\sum_{y=1}^{\infty} M_{L,P+y} N_{L,P-y}$ can be symmetrized. Indeed, we can write

$$\sum_{y=1}^{\infty} X_{L+1,P+y} X_{L+1,P-y+1} = \sum_{z=-\infty}^{0} X_{L+1,P-z+1} X_{L+1,P+z} = \frac{1}{2} \sum_{k=-\infty}^{\infty} X_{L+1,P+k} X_{L+1,P-k+1} \tag{C9}$$

where the first equality is obtained by setting $z = 1 - y$ and the second equality results from the fact that the sums over y and z add up to the (complete) sum over the whole range of k, remembering that y, z and k are dummy variables. Similarly, we have

$$\sum_{y=1}^{\infty} X_{L+1,P+y+1} X_{L+1,P-y+1} = \frac{1}{2} \sum_{y=-\infty}^{\infty} X_{L+1,P+y+1} X_{L+1,P-y+1} - \frac{1}{2} X_{L+1,P+1}^2 \tag{C10}$$

$$\sum_{y=1}^{\infty} X_{L+1,P+y} X_{L+1,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} X_{L+1,P+y} X_{L+1,P-y} - \frac{1}{2} X_{L+1,P}^2 \tag{C11}$$

$$\sum_{y=1}^{\infty} X_{L+1,P+y+1} X_{L+1,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} X_{L+1,P+y+1} X_{L+1,P-y} - X_{L+1,P} X_{L+1,P+1}. \tag{C12}$$

The proof of these equalities is similar to that of equation (C9), though we must be careful about the boundary terms. Now, from equations (C8) to (C12), we deduce that

$$\begin{aligned}
\sum_{y=1}^{\infty} & M_{L,P+y} N_{L,P-y} \\
&= \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L,P+y} N_{L,P-y} + \frac{(\alpha\beta)^2}{2} \left(a X_{L+1,P+1}^2 + b X_{L+1,P}^2 - 2 X_{L+1,P} X_{L+1,P+1} \right) \\
&= -\frac{\alpha\beta}{2} X_{2L+2,2P+1} + \frac{\alpha\beta}{2} (N_{L,P} X_{L+1,P+1} + M_{L,P} X_{L+1,P}) \\
&= -\frac{\alpha\beta}{2} X_{2L+2,2P+1} - \frac{1}{2(1-ab)} \left(b N_{L,P}^2 + 2 M_{L,P} N_{L,P} + a M_{L,P}^2 \right)
\end{aligned} \tag{C13}$$

where the second equality results from equations (C5), (A4) and (A5) and the last equality results from equation (A3).

Differentiating equation (C13) with respect to a we obtain

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y} N_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y} N_{L,P-y} + \alpha\beta X_{L+1,P} \tilde{M}_{L,P} - \frac{\alpha^2\beta^2}{2} X_{L+1,P+1}^2. \tag{C14}$$

In the following calculations, we shall need an equivalent form for equation (C14), obtained by writing $\tilde{M}_{L,P} = \frac{1}{\alpha} \tilde{M}_{L-1,P} + M_{L-1,P}$ (see equation (A7)) and expressing $M_{L-1,P}$ as a function of X (see equation (A4)):

$$\begin{aligned}
\sum_{y=1}^{\infty} \tilde{M}_{L,P+y} N_{L,P-y} &= \frac{1}{2} \sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y} N_{L,P-y} + \beta X_{L+1,P} \tilde{M}_{L-1,P} \\
&\quad - \frac{\alpha^2\beta^2}{2} \left(X_{L+1,P+1}^2 - \frac{2}{\beta} X_{L+1,P} X_{L,P} + 2 X_{L+1,P+1} X_{L+1,P} \right).
\end{aligned} \tag{C15}$$

Now, deriving equation (C13) with respect to b, we obtain

$$\sum_{y=1}^{\infty} M_{L,P+y} \tilde{N}_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L,P+y} \tilde{N}_{L,P-y} + \alpha\beta X_{L+1,P+1} \tilde{N}_{L,P} - \frac{\alpha^2\beta^2}{2} X_{L+1,P}^2. \tag{C16}$$

Using a procedure similar to that used to derive equation (C13), we calculate the sum

$$\sum_{y=1}^{\infty} M_{L,P+y+1} N_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L,P+y+1} N_{L,P-y} + \frac{\alpha\beta}{2} (1 - \alpha - \beta) X_{L+1,P+1}^2. \tag{C17}$$

Deriving equation (C17) with respect to a and b, we obtain

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y-1} N_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y-1} N_{L,P-y} + \alpha\beta X_{L+1,P} \tilde{M}_{L,P-1} - \frac{\alpha^2\beta(1-\beta)}{2} X_{L+1,P}^2 \tag{C18}$$

$$\sum_{y=1}^{\infty} M_{L,P+y} \tilde{N}_{L,P-y+1} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L,P+y} \tilde{N}_{L,P-y+1} + \alpha\beta X_{L+1,P+1} \tilde{N}_{L,P+1} - \frac{\alpha(1-\alpha)\beta^2}{2} X_{L+1,P+1}^2 \tag{C19}$$

$$= \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L,P+y} \tilde{N}_{L,P-y+1} + \alpha X_{L+1,P+1} \tilde{N}_{L-1,P} - \frac{(\alpha\beta)^2}{2} X_{L+1,P+1} \left(X_{L+1,P+1} + \frac{X_{L,P} - X_{L,P+1}}{\alpha} \right). \tag{C20}$$

The last equality was obtained by using $\tilde{N}_{L,P+1} = \tilde{N}_{L-1,P}/\beta + N_{L-1,P}$ (equation (A8)) and expressing $N_{L-1,P}$ as a function of X from equation (A5).

The twelve sums that appear in equation (66) can now be calculated using equations (C13) to (C20) and we obtain

$$\sum_{y=1}^{\infty} M_{L-1,P+y} \tilde{N}_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L-1,P+y} \tilde{N}_{L,P-y} + \alpha\beta X_{L,P+1} \tilde{N}_{L,P} - \frac{\alpha^2\beta^2}{2} \left(X_{L+1,P}^2 - \frac{1-\alpha}{\alpha} X_{L,P}^2 - X_{L,P-1}^2 \right) \tag{C21}$$

$$\sum_{y=1}^{\infty} M_{L-1,P+y} \tilde{N}_{L,P-y+1} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L-1,P+y} \tilde{N}_{L,P-y+1} + \alpha X_{L,P+1} \tilde{N}_{L-1,P} - \frac{\alpha^2\beta^2}{2} \left(X_{L+1,P+1}^2 - \frac{1}{\alpha} X_{L,P+1}^2 \right) \tag{C22}$$

$$\sum_{y=1}^{\infty} M_{L-1,P+y-1} \tilde{N}_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L-1,P+y-1} \tilde{N}_{L,P-y} + \alpha\beta X_{L,P} \tilde{N}_{L,P} - \frac{\alpha^2\beta^2}{2} \left(\frac{1-\alpha}{\alpha} X_{L,P}^2 + X_{L,P-1}^2 \right) \tag{C23}$$

$$\sum_{y=1}^{\infty} M_{L-1,P+y-1} \tilde{N}_{L,P-y+1} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L-1,P+y-1} \tilde{N}_{L,P-y+1} + \alpha X_{L,P} \tilde{N}_{L-1,P} - \frac{\alpha^2\beta^2}{2} \frac{X_{L,P}^2}{\alpha} \tag{C24}$$

$$\sum_{y=1}^{\infty} M_{L-2,P+y-1} \tilde{N}_{L,P-y} = \frac{1}{2} \sum_{y=-\infty}^{\infty} M_{L-2,P+y-1} \tilde{N}_{L,P-y} + \alpha\beta X_{L-1,P} \tilde{N}_{L,P} - \frac{\alpha^2\beta^2}{2} \left(\frac{1-\alpha}{\alpha} \left(X_{L-1,P}^2 - X_{L-1,P-1}^2 \right) + 2 X_{L,P-1} X_{L-1,P-1} \right) \tag{C25}$$

$$\sum_{y=1}^{\infty} M_{L-2,P+y-1}\tilde{N}_{L,P-y+1} = \frac{1}{2}\sum_{y=-\infty}^{\infty} M_{L-2,P+y-1}\tilde{N}_{L,P-y+1} + \alpha X_{L-1,P}\tilde{N}_{L-1,P} - \frac{\alpha^2\beta^2}{2}X_{L,P}^2 \tag{C26}$$

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y}N_{L-1,P-y} = \frac{1}{2}\sum_{y=-\infty}^{\infty} \tilde{M}_{L-1,P+y}N_{L,P-y} + \beta X_{L,P}\tilde{M}_{L-1,P} - \frac{\alpha^2\beta^2}{2}\left(X_{L+1,P+1}^2 - \frac{1}{\beta}X_{L,P}^2\right) \tag{C27}$$

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y-1}N_{L-1,P-y} = \frac{1}{2}\sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y-1}N_{L-1,P-y} + \alpha\beta X_{L,P}\tilde{M}_{L,P-1} - \frac{\alpha^2\beta^2}{2}\left(\frac{1-\beta}{\beta}(X_{L+1,P}^2 - X_{L,P-1}^2) - X_{L,P}^2\right) \tag{C28}$$

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y}N_{L-1,P-y-1} = \frac{1}{2}\sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y}N_{L-1,P-y-1} + \beta X_{L,P-1}\tilde{M}_{L-1,P} - \frac{\alpha^2\beta}{2}\left(X_{L,P}^2 - 2X_{L,P}X_{L+1,P} + 2\beta X_{L+1,P}X_{L+1,P+1}\right) \tag{C29}$$

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y-1}N_{L-1,P-y-1} = \frac{1}{2}\sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y-1}N_{L-1,P-y-1} + \alpha\beta X_{L,P-1}\tilde{M}_{L,P-1} - \frac{\alpha^2\beta^2}{2}\left(X_{L,P}^2 + \frac{1-\beta}{\beta}X_{L,P-1}^2\right) \tag{C30}$$

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y}N_{L-2,P-y-1} = \frac{1}{2}\sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y}N_{L-2,P-y-1} + \beta X_{L-1,P-1}\tilde{M}_{L-1,P} - \frac{\alpha^2\beta^2}{2}\left(-\frac{1-\beta}{\beta}X_{L,P}^2 + 2X_{L,P}X_{L,P+1}\right) \tag{C31}$$

$$\sum_{y=1}^{\infty} \tilde{M}_{L,P+y-1}N_{L-2,P-y-1} = \frac{1}{2}\sum_{y=-\infty}^{\infty} \tilde{M}_{L,P+y-1}N_{L-2,P-y-1} + \alpha\beta X_{L-1,P-1}\tilde{M}_{L,P-1} - \frac{\alpha^2\beta^2}{2}\left(X_{L-1,P}^2 + 2\frac{1-\beta}{\beta}X_{L-1,P-1}X_{L,P-1} - X_{L-1,P-1}^2\right). \tag{C32}$$

All the twelve sums (C21) to (C32) have a similar structure that is composed of three parts: (i) $\frac{1}{2}$ times the complete sum, that ranges from $-\infty$ to ∞; (ii) a term made of a product of an X function with an $\tilde{M}$ or an $\tilde{N}$; (iii) a quadratic term in X. We shall show that when we substitute these sums in the formula (66) for the diffusion constant, only the complete sums contribute to the final result, i.e. the contribution of the terms of type (ii) vanishes identically and the contribution of the terms of type (iii) cancels out with the first term on the right-hand side of equation (66).

We start with the terms of type (ii). In equation (66) there are two distinct parts, the first one with coefficient c_n and the other one with coefficient c_m. These two parts can be treated separately. We consider the 'c_n part' and evaluate, first of all, the contribution of the terms of type (ii) i.e. containing an $\tilde{N}$ factor; we find

$$\alpha X_{L+1,P}\tilde{N}_{L-1,P}(Z_{L,P}X_{L-1,P} - Z_{L-1,P}X_{L,P} - Z_{L-1,P-1}X_{L,P+1}) - \alpha\beta X_{L+1,P+1}\tilde{N}_{L,P} \times (Z_{L,P}X_{L-1,P} - Z_{L-1,P}X_{L,P} - Z_{L-1,P-1}X_{L,P+1}) = 0 \tag{C33}$$

where the term within braces vanishes thanks to equation (A9). Similarly, the terms of type (ii) multiplied by c_m (i.e. those containing an $\tilde{M}$ factor) cancel out.

We now study the contribution to expression (66) of the terms quadratic in X. Collecting all the terms and leaving aside, for the time being, the global factor $\frac{\alpha^2\beta^2}{2}$, we find

$$-Z_{L,P}\Big\{X_{L+1,P}X_{L,P}^2 - X_{L+1,P+1}\big(-X_{L-1,P}^2 + 2X_{L,P-1}X_{L-1,P-1} + X_{L-1,P-1}^2\big) - \frac{1}{\alpha}X_{L+1,P+1} \times \big(X_{L-1,P}^2 - X_{L-1,P-1}^2\big)\Big\} + Z_{L-1,P}\Big\{- X_{L+1,P+1}\big(X_{L,P-1}^2 - X_{L,P}^2\big) + \frac{1}{\alpha}X_{L,P}^2 \times (X_{L+1,P} - X_{L+1,P+1})\Big\} + Z_{L-1,P-1}\Big\{X_{L+1,P}X_{L+1,P+1}^2 - X_{L+1,P+1} \times \big(X_{L+1,P}^2 + X_{L,P}^2 - X_{L,P-1}^2\big) + \frac{1}{\alpha}\big(X_{L+1,P+1}X_{L,P}^2 - X_{L+1,P}X_{L,P+1}^2\big)\Big\}. \quad \text{(C34)}$$

Here we have two categories of terms: terms with a multiplicative factor $1/\alpha$ and terms without the multiplicative factor $1/\alpha$. We first simplify the terms in expression (C34) that are not multiplied by $1/\alpha$; writing, from Pascal's relations, $2X_{L-1,P-1} = X_{L,P} + X_{L-1,P-1} - X_{L-1,P}$ and $X_{L-1,P-1}^2 - X_{L-1,P}^2 = X_{L,P}[X_{L-1,P-1} - X_{L-1,P}]$, we find

$$\begin{aligned}
&-Z_{L,P}\big\{X_{L+1,P}X_{L,P}^2 - X_{L+1,P+1}(X_{L,P}[X_{L-1,P-1} - X_{L-1,P}] + X_{L,P-1}[X_{L,P} + X_{L-1,P-1} \\
&\quad -X_{L-1,P}])\big\} + Z_{L-1,P}X_{L+1,P+1}X_{L+1,P}(X_{L,P} - X_{L,P-1}) \\
&\quad + Z_{L-1,P-1}X_{L+1,P+1}\big(X_{L+1,P}X_{L+1,P+1} - X_{L+1,P}^2 - X_{L,P}^2 + (X_{L+1,P} - X_{L,P})^2\big) \\
&= -Z_{L,P}\big(X_{L+1,P}X_{L,P}^2 - X_{L+1,P+1}X_{L,P-1}X_{L,P} - X_{L+1,P+1}X_{L+1,P}(X_{L-1,P-1} \\
&\quad -X_{L-1,P})\big) + X_{L+1,P+1}X_{L+1,P}(Z_{L-1,P}(X_{L,P} - X_{L,P-1}) + Z_{L-1,P-1}(X_{L+1,P+1} \\
&\quad -2X_{L,P})) \\
&= -Z_{L,P}X_{L,P}(X_{L+1,P}X_{L,P} - X_{L+1,P+1}X_{L,P-1}) + X_{L+1,P+1}X_{L+1,P} \\
&\quad \times\{Z_{L,P}(X_{L-1,P-1} - X_{L-1,P}) + Z_{L-1,P}(X_{L,P} - X_{L,P-1}) \\
&\quad + Z_{L-1,P-1}(X_{L,P+1} - X_{L,P})\}.
\end{aligned} \quad \text{(C35)}$$

The expression within the braces in the last equality vanishes identically, thanks to equations (A9) and (A10). Using the first equality in equation (A6), we find that expression (C35) (multiplied by the factor $\frac{\alpha^2\beta^2}{2}$ that was left aside while writing equation (C34)) reduces to

$$-\frac{\alpha\beta Z_{L,P}^2}{2(\alpha+\beta-1)}X_{L,P}. \quad \text{(C36)}$$

We now simplify the terms in equation (C34) that have the multiplicative factor $1/\alpha$:

$$\begin{aligned}
&\frac{Z_{L,P}}{\alpha}X_{L+1,P+1}X_{L,P}(X_{L-1,P} - X_{L-1,P-1}) + \frac{Z_{L-1,P}}{\alpha}X_{L,P}(X_{L+1,P}(X_{L+1,P+1} - X_{L,P+1}) \\
&\quad - X_{L+1,P+1}(X_{L+1,P} - X_{L,P-1})) + \frac{Z_{L-1,P-1}}{\alpha}\big(X_{L+1,P+1}X_{L,P}^2 - X_{L+1,P}X_{L,P+1}^2\big) \\
&= \frac{Z_{L,P}}{\alpha}X_{L+1,P+1}X_{L,P}(X_{L-1,P} - X_{L-1,P-1}) + \frac{1}{\alpha}(X_{L+1,P+1}X_{L,P}(Z_{L-1,P}X_{L,P-1} \\
&\quad + Z_{L-1,P-1}X_{L,P}) - X_{L+1,P}X_{L,P+1}(Z_{L-1,P}X_{L,P} + Z_{L-1,P-1}X_{L,P+1})) \\
&= \frac{Z_{L,P}}{\alpha}(X_{L+1,P+1}X_{L,P}(X_{L-1,P} - X_{L-1,P-1}) + X_{L+1,P+1}X_{L,P}X_{L-1,P-1} \\
&\quad - X_{L+1,P}X_{L,P+1}X_{L-1,P}) \\
&= \frac{Z_{L,P}}{\alpha}X_{L-1,P}(X_{L+1,P+1}X_{L,P} - X_{L+1,P}X_{L,P+1})
\end{aligned} \quad \text{(C37)}$$

where the last but one equality is obtained with the help of equations (A9) and (A10). Using the third equality in equation (A6), we find that expression (C37), multiplied by the factor $\frac{\alpha^2\beta^2}{2}$ left aside while writing equation (C34), is equal to

$$\frac{\alpha\beta Z_{L,P}^2}{2(\alpha+\beta-1)}\frac{X_{L-1,P}}{\alpha}. \tag{C38}$$

Adding the two terms (C36) and (C38), and inserting the result in equation (66) we obtain

$$\frac{2(\alpha+\beta-1)}{Z_{L,P}^2}c_n\frac{Z_{L,P}^2}{2(\alpha+\beta-1)}(\beta X_{L-1,P}-\alpha\beta X_{L,P}) = -\frac{M_{L,P}N_{L-2,P-1}}{Z_{L,P}} \tag{C39}$$

where we have used equation (A5) and the expression of c_n (equation (42)); this term cancels out exactly the term $M_{L,P}N_{L-2,P-1}/Z_{L,P}$ appearing in equation (66).

In the same manner, the contribution of the terms quadratic in X that are multiplied by c_m exactly cancels out the term $N_{L,P}M_{L-2,P-1}/Z_{L,P}$ appearing in equation (66).

Hence, expression (66) of the diffusion constant reduces to

$$\begin{aligned}\Delta = \frac{(\alpha+\beta-1)}{Z_{L,P}^2}\sum_{y=-\infty}^{\infty}\{&c_n(Z_{L,P}M_{L-2,P+y-1}-Z_{L-1,P}M_{L-1,P+y-1}-Z_{L-1,P-1}M_{L-1,P+y})\\ &\times(X_{L+1,P}\tilde{N}_{L,P-y+1}-X_{L+1,P+1}\tilde{N}_{L,P-y})+c_m(Z_{L,P}N_{L-2,P-y-1}\\ &-Z_{L-1,P}N_{L-1,P-y-1}-Z_{L-1,P-1}N_{L-1,P-y})(X_{L+1,P}\tilde{M}_{L,P+y}\\ &-X_{L+1,P+1}\tilde{M}_{L,P+y-1})\}.\end{aligned} \tag{C40}$$

In this equation, the summation variable y runs from $-\infty$ to ∞ and the sums are calculated using formulae (C6) and (C7). We substitute the expressions for the sums in equation (C40) and group together the terms which have the common multiplicative factor $Z_{L,P}$, $Z_{L-1,P}$ or $Z_{L-1,P-1}$. After some simplifications, we obtain the final expression (67).

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