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Exact Diffusion Constant of a One-Dimensional Asymmetric Exclusion Model with Open Boundaries

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For the 1D fully asymmetric exclusion model with open boundary conditions, we calculate exactly the fluctuations of the current of particles. The method used is an extension of a matrix technique developed recently to describe the equal-time steady-state properties for open boundary conditions and the diffusion constant for particles on a ring. We show how the fluctuations of the current are related to non-equal-time correlations. In the thermodynamic limit, our results agree with recent results of Ferrari and Fontes obtained by working directly in the infinite system. We also show that the fluctuations of the current become singular when the system undergoes a phase transition with discontinuities along the first-order transition line.

KEY WORDS: Stochastic lattice gas; asymmetric exclusion; diffusion constant.

1. INTRODUCTION

The one-dimensional asymmetric simple exclusion process (ASEP)[1-3] is one of the simplest examples of a stochastic system out of equilibrium.[4,5] It describes a driven lattice gas with hard-core repulsion; it can also be related to hopping conductivity,[6] growth processes,[7,8] traffic jams or queuing models,[9] and the problem of directed polymers in random media.[10,11]

The steady-state of the fully asymmetric exclusion process is known exactly[12-15] in one dimension. For periodic boundary conditions,[12] the

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stationary state is simple: all configurations have equal probabilities. For open boundary conditions, the steady-state is more complicated[13]; nevertheless it was shown that the stationary weight of a configuration can be expressed as a product of noncommuting matrices.[14] With such a matrix method, arbitrary equal-time correlation functions in the steady-state can be computed. Exact expressions of the density profile and the current have been obtained for arbitrary input and output rates (α and β) at the two ends of the system and for arbitrary system sizes. In the limit of infinite systems, the expression of the current becomes nonanalytic across some lines in the α–β plane separating the phase diagram into three regions: a low-density phase, a high-density phase, and a maximal current phase.[13–16]

Non-steady-state properties[17] or unequal-time correlation functions in the steady-state[18] are much harder to compute for this model. The eigenvalues of the master equation can be determined by a Bethe Ansatz[19,20]; however, the eigenvectors are complicated enough that the expressions of unequal-time correlations remain very difficult to obtain. Several physical quantities can be expressed in terms of these correlation functions, in particular the variance of the number of particles that flow through a marked bond in the system. This variance increases linearly with time. The rate of increase is a quantity Δ which can be interpreted as a diffusion constant.[21] The goal of this paper is to calculate exactly this diffusion constant for the ASEP in one dimension with open boundary conditions.

In a recent work, an exact expression for the diffusion constant of a marked particle has been obtained using a matrix formulation[22] for all lattice sizes and all possible numbers of particles for the ASEP with periodic boundary conditions.

In the present paper, we extend this approach to calculate a similar quantity Δ in the case of open boundary conditions. The solution obtained here is more intricate than in the periodic case, as the steady-state itself has a more complex structure. In particular it involves matrices the elements of which are themselves matrices. We will show that in the maximal current phase, Δ vanishes in the thermodynamic limit, whereas it has a nonzero limit in the other two phases. Also, Δ exhibits singularities at the phase boundaries. As a by-product of our calculation, we also obtain exact expressions of the time integrals of some unequal-time correlation functions.

The paper is organized as follows: in Section 2 we derive an expression for Δ in terms of quantities $s(\mathscr{C})$ which in Section 3 we calculate using an extension of the matrix technique; in Section 4 we present numerical and exact calculations of Δ and in Section 5 we discuss the relation to non-equal-time correlation functions; we conclude in Section 6.

Let us first recall the dynamics of the one-dimensional exclusion model with open boundary conditions. Each site i ($1 \leqslant i \leqslant N$) of a one-dimensional lattice of N sites is either occupied by a particle ($\tau_i = 1$) or empty ($\tau_i = 0$). During every infinitesimal time interval dt, each particle in the system has a probability dt of jumping to the next site on its right (for all particles on sites $1 \leqslant i \leqslant N-1$) if this neighboring site is empty. Furthermore, a particle is added at site $i = 1$ with probability $\alpha\, dt$ if site 1 is empty and a particle is removed from site N with probability $\beta\, dt$ if this site is occupied.

In the long-time limit, the system reaches a steady-state. In the steady-state it has been shown[14] that the probability $p(\mathscr{C})$ of finding in configuration $\mathscr{C} = \{\tau_1, \tau_2, ..., \tau_N\}$ can be expressed as

$$p(\mathscr{C}) = \frac{1}{Z_N} \langle\alpha| \prod_{i=1}^{N} (\tau_i D + (1-\tau_i) E) |\beta\rangle \tag{1}$$

where D and E are matrices and $\langle\alpha|$ and $|\beta\rangle$ are vectors satisfying the following algebraic rules:

$$\begin{aligned} DE &= D + E \\ D\,|\beta\rangle &= \frac{1}{\beta}\,|\beta\rangle \\ \langle\alpha|\, E &= \frac{1}{\alpha}\,\langle\alpha| \end{aligned} \tag{2}$$

The normalization Z_N is given by

$$Z_N = \langle\alpha|\, C^N\, |\beta\rangle \tag{3}$$

where

$$C = DE = D + E \tag{4}$$

It was shown in ref. 14 that noncommuting matrices which satisfy (2) have to be of infinite dimension. (Only in the special case $\alpha + \beta = 1$ can D and E be chosen to be one dimensional, $D = 1/\beta$ and $E = 1/\alpha$.) Several representations of (2) are possible,[14] for example,

$$D = \begin{pmatrix} 1/\beta & 1/\beta & 1/\beta & 1/\beta & \cdot & \cdot \\ 0 & 1 & 1 & 1 & & \\ 0 & 0 & 1 & 1 & & \\ 0 & 0 & 0 & 1 & & \\ \cdot & & & & & \cdot \\ \cdot & & & & & \cdot \end{pmatrix}, \qquad E = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & 0 & 0 & 0 & & \\ 0 & 1 & 0 & 0 & & \\ 0 & 0 & 1 & 0 & & \\ \cdot & & & \cdot & & \\ \cdot & & & & & \cdot \end{pmatrix} \tag{5}$$

$$\langle\alpha| = (1, (1/\alpha), (1/\alpha)^2 \quad \cdot \quad \cdot), \qquad |\beta\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \cdot \\ \cdot \end{pmatrix} \tag{6}$$

2. THE MASTER EQUATION AND ITS CONSEQUENCES

The main quantity we consider in this paper is the total number of particles having entered the system up to time t. Let us call this number Y_t. In the long-time limit, the current J of particles entering the system is constant; it is simply the probability that the first site is empty in the stationary state multiplied by α, the rate at which particles attempt to enter the system. Thus, using the algebraic rules (2), we have

$$J = \alpha \frac{\langle\alpha| EC^{N-1} |\beta\rangle}{\langle\alpha| C^N |\beta\rangle} = \frac{\langle\alpha| C^{N-1} |\beta\rangle}{\langle\alpha| C^N |\beta\rangle} \tag{7}$$

If $\langle \cdot \rangle$ denotes an average over the history of the dynamics and steady-state initial conditions, one has

$$\frac{1}{t} \langle Y_t \rangle = J \tag{8}$$

Our aim is to study the fluctuations of Y_t. We shall show that in the long-time limit,

$$\frac{\langle Y_t^2 \rangle - \langle Y_t \rangle^2}{t} \to \Delta \tag{9}$$

where Δ is a quantity of the same nature as the diffusion constant in ref. 22 and is related to non-equal-time correlations (see Section 5).

Let $P_t(Y, \mathscr{C} \mid \mathscr{C}_0)$ be the probability that the system is in configuration $\mathscr{C}$ at time t and that $Y_t = Y$, given that at time $t = 0$ the configuration was $\mathscr{C}_0$. The time evolution of $P_t(Y, \mathscr{C} \mid \mathscr{C}_0)$ can be written in the following form:

$$\begin{aligned} \frac{d}{dt} P_t(Y, \mathscr{C} \mid \mathscr{C}_0) &= \sum_{\mathscr{C}_1 \neq \mathscr{C}_0} [P_t(Y, \mathscr{C} \mid \mathscr{C}_1) - P_t(Y, \mathscr{C} \mid \mathscr{C}_0)]\, M_0(\mathscr{C}_1, \mathscr{C}_0) \\ &\quad + [P_t(Y-1, \mathscr{C} \mid \mathscr{C}_1) - P_t(Y, \mathscr{C} \mid \mathscr{C}_0)]\, M_1(\mathscr{C}_1, \mathscr{C}_0) \end{aligned} \tag{10}$$

where $M_0(\mathscr{C}_1, \mathscr{C}_0)\,dt$ is the probability of going from $\mathscr{C}_0$ to $\mathscr{C}_1$ without adding a particle at site 1, and $M_1(\mathscr{C}_1, \mathscr{C}_0)\,dt$ is the probability of going from $\mathscr{C}_0$ to $\mathscr{C}_1$ by adding a particle at site 1, in a time interval dt. If one then defines

$$M_0(\mathscr{C}_0, \mathscr{C}_0) = -\sum_{\mathscr{C}_1 \neq \mathscr{C}_0} [M_0(\mathscr{C}_1, \mathscr{C}_0) + M_1(\mathscr{C}_1, \mathscr{C}_0)]$$

Eq. (10) becomes

$$\frac{d}{dt} P_t(Y, \mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}_1} P_t(Y, \mathscr{C} \mid \mathscr{C}_1)\, M_0(\mathscr{C}_1, \mathscr{C}_0) + P_t(Y-1, \mathscr{C} \mid \mathscr{C}_1)\, M_1(\mathscr{C}_1, \mathscr{C}_0) \tag{11}$$

The continuous-time transition matrix of the ASEP is given by

$$M(\mathscr{C}', \mathscr{C}) = M_0(\mathscr{C}', \mathscr{C}) + M_1(\mathscr{C}', \mathscr{C})$$

It has the two essential properties

$$\sum_{\mathscr{C}'} M(\mathscr{C}', \mathscr{C}) = 0 \tag{12}$$

$$\sum_{\mathscr{C}} M(\mathscr{C}', \mathscr{C})\, p(\mathscr{C}) = 0 \tag{13}$$

Equation (12) expresses the conservation of probability and (13) the fact that the $p(\mathscr{C})$ are the steady-state weights. Let us define the following two quantities:

$$p_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{Y} P_t(Y, \mathscr{C} \mid \mathscr{C}_0) \quad \text{and} \quad q_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{Y} P_t(Y, \mathscr{C} \mid \mathscr{C}_0)\, Y \tag{14}$$

The equations satisfied by $p_t(\mathscr{C} \mid \mathscr{C}_0)$ and $q_t(\mathscr{C} \mid \mathscr{C}_0)$ can be found by appropriately summing (11),

$$\frac{d}{dt} p_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}_1} p_t(\mathscr{C} \mid \mathscr{C}_1)\, M(\mathscr{C}_1, \mathscr{C}_0) \tag{15}$$

$$\frac{d}{dt} q_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}_1} q_t(\mathscr{C} \mid \mathscr{C}_1)\, M(\mathscr{C}_1, \mathscr{C}_0) + \sum_{\mathscr{C}_1} p_t(\mathscr{C} \mid \mathscr{C}_1)\, M_1(\mathscr{C}_1, \mathscr{C}_0) \tag{16}$$

In the long-time limit, one can show (see Appendix A) that their asymptotic behavior is given by[23]

$$p_t(\mathscr{C} \mid \mathscr{C}_0) \to p(\mathscr{C}) \tag{17}$$

$$q_t(\mathscr{C} \mid \mathscr{C}_0) - Jp(\mathscr{C})\, t \to r(\mathscr{C}) + p(\mathscr{C})\, s(\mathscr{C}_0) \tag{18}$$

The average of Y_t given that the initial configuration was $\mathscr{C}_0$ is

$$\langle Y_t \mid \mathscr{C}_0 \rangle = \sum_{\mathscr{C}} q_t(\mathscr{C} \mid \mathscr{C}_0) \simeq Jt + \sum_{\mathscr{C}} r(\mathscr{C}) + s(\mathscr{C}_0) \tag{19}$$

For large t, one sees from (19) that the leading behavior is determined by the steady-state current, which does not depend on $\mathscr{C}_0$, but the memory $s(\mathscr{C}_0)$ of the initial configuration is kept in the subdominant term, which does not grow with t.

By multiplying the two sides of (11) by $p(\mathscr{C}_0)$ and Y or Y^2, summing over $\mathscr{C}_0$, $\mathscr{C}$, and Y, and using (13), we obtain the equations for the time derivatives of the first two moments of Y_t,

$$\frac{d}{dt} \langle Y_t \rangle = \sum_{\mathscr{C}_0, \mathscr{C}_1} M_1(\mathscr{C}_1, \mathscr{C}_0)\, p(\mathscr{C}_0) \tag{20}$$

$$\frac{d}{dt} \langle Y_t^2 \rangle = 2 \sum_{\mathscr{C}, \mathscr{C}_0, \mathscr{C}_1} q_t(\mathscr{C} \mid \mathscr{C}_1)\, M_1(\mathscr{C}_1, \mathscr{C}_0)\, p(\mathscr{C}_0) + \sum_{\mathscr{C}_0, \mathscr{C}_1} M_1(\mathscr{C}_1, \mathscr{C}_0)\, p(\mathscr{C}_0) \tag{21}$$

Equation (20) provides an expression for the current

$$J = \sum_{\mathscr{C}_0, \mathscr{C}_1} M_1(\mathscr{C}_1, \mathscr{C}_0)\, p(\mathscr{C}_0) \tag{22}$$

Combining (20) and (21), we can write the time evolution of the fluctuations of Y_t as follows:

$$\begin{aligned} \frac{d}{dt} (\langle Y_t^2 \rangle - \langle Y_t \rangle^2) &= \frac{d}{dt} \langle Y_t^2 \rangle - 2 \langle Y_t \rangle \frac{d}{dt} \langle Y_t \rangle \\ &= 2 \sum_{\mathscr{C}, \mathscr{C}_0, \mathscr{C}_1} q_t(\mathscr{C} \mid \mathscr{C}_1)\, M_1(\mathscr{C}_1, \mathscr{C}_0)\, p(\mathscr{C}_0) + J - 2J \sum_{\mathscr{C}, \mathscr{C}_0} q_t(\mathscr{C} \mid \mathscr{C}_0)\, p(\mathscr{C}_0) \end{aligned} \tag{23}$$

Inserting in both sides of this equation the expected long-time behavior (9), (17), and (18), one obtains the expressions of the diffusion constant in terms of $s(\mathscr{C})$,

$$\Delta = J + 2 \sum_{\mathscr{C},\mathscr{C}'} s(\mathscr{C})\, M_1(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}') - 2J \sum_{\mathscr{C}} s(\mathscr{C})\, p(\mathscr{C}) \tag{24}$$

Similarly, by substituting the asymptotic behavior (18) into Eq. (16), one obtains the equation satified by $s(\mathscr{C})$,

$$\sum_{\mathscr{C}_1} s(\mathscr{C}_1)\, M(\mathscr{C}_1, \mathscr{C}_0) = J - \sum_{\mathscr{C}_1} M_1(\mathscr{C}_1, \mathscr{C}_0) \tag{25}$$

Hence, to obtain Δ, it is sufficient to calculate the $s(\mathscr{C})$. But, due to (12), the solution $s(\mathscr{C})$ of (25) can only be obtained up to a constant. It is easy to check, however, by using the expression (22) for the current, that the addition of the same constant to all the $s(\mathscr{C})$ does not affect the value (24) of Δ. In the next section, we shall obtain an exact solution of (25) by using an extension of the matrix formalism.

Remark 1. *Discrete-time dynamics.* One can also consider the ASEP under discrete-time dynamics, in which case at each time step one of the $N+1$ bonds is randomly chosen and updated (where bond 0 is on the left of the first site and bond N is on the right of the Nth site).[13] One can define a current $J^{(d)}$ and diffusion constant $\Delta^{(d)}$ in terms of the moments of Y_T, the number of particles which have entered the system after T updates:

$$\begin{aligned} \langle Y_T \rangle &\to J^{(d)} T \\ \langle Y_T^2 \rangle - \langle Y_T \rangle^2 &\to \Delta^{(d)} T \end{aligned} \tag{26}$$

In the case of discrete-time dynamics the evolution of the probabilities $p_T(\mathscr{C} \mid \mathscr{C}_0)$, for example, is given by

$$p_{T+1}(\mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}_1} p_T(\mathscr{C} \mid \mathscr{C}_1)\, M^{(d)}(\mathscr{C}_1, \mathscr{C}_0) \tag{27}$$

where $M^{(d)} = M_0^{(d)} + M_1^{(d)}$ is the transition matrix for discrete time and is related to $M = M_0 + M_1$, the transition matrix for continuous time, by

$$\begin{aligned} M_0^{(d)}(\mathscr{C}_1, \mathscr{C}_0) &= \delta_{\mathscr{C}_1, \mathscr{C}_0} + \frac{1}{N+1} M_0(\mathscr{C}_1, \mathscr{C}_0) \\ M_1^{(d)}(\mathscr{C}_1, \mathscr{C}_0) &= \frac{1}{N+1} M_1(\mathscr{C}_1, \mathscr{C}_0) \end{aligned} \tag{28}$$

Modifying the steps leading from (15)–(25) and using (28), one finds that the $s(\mathscr{C})$ satisfy the same equation (25) as in the continuous-time case. This leads to the following expression for the discrete-time current and diffusion constant in terms of the continuous-time expressions:

$$J^{(d)} = \frac{J}{N+1}$$

$$\Delta^{(d)} = \frac{\Delta}{N+1} - \left[\frac{J}{N+1}\right]^2$$

Remark 2. Equation (11) was obtained by decomposing the time interval $[0, t+dt]$ into two subintervals $[0, dt]$ and $[dt, t+dt]$. If instead it were decomposed into $[0, t]$ and $[t, t+dt]$, one would obtain

$$\frac{d}{dt} P_t(Y, \mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}'} M_0(\mathscr{C}, \mathscr{C}')\, P_t(Y, \mathscr{C}' \mid \mathscr{C}_0) + M_1(\mathscr{C}, \mathscr{C}')\, P_t(Y-1, \mathscr{C}' \mid \mathscr{C}_0)$$

and, as in ref. 22, an expression for Δ would be obtained in terms of the quantities $r(\mathscr{C})$ which appear in (18),

$$\Delta = J + 2 \sum_{\mathscr{C}, \mathscr{C}'} M_1(\mathscr{C}, \mathscr{C}')\, r(\mathscr{C}') - 2J \sum_{\mathscr{C}} r(\mathscr{C}) \tag{29}$$

Clearly, the result obtained for Δ must be the same. The $r(\mathscr{C})$ would satisfy an inhomogeneous linear equation

$$\sum_{\mathscr{C}'} M(\mathscr{C}, \mathscr{C}')\, r(\mathscr{C}') = Jp(\mathscr{C}) - \sum_{\mathscr{C}'} M_1(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}') \tag{30}$$

The $r(\mathscr{C})$ are determined by this equation only up to the addition of a multiple of $p(\mathscr{C})$ that does not affect the value of Δ. For general α and β we did not succeed in finding exact expressions for the $r(\mathscr{C})$, solution of (30). However, along the line $\alpha + \beta = 1$, it can be checked that Eq. (30) is satisfied by

$$r(\mathscr{C}) = \alpha\beta \frac{dp(\mathscr{C})}{d\alpha} \tag{31}$$

3. SOLUTION FOR $s(\mathscr{C})$ IN TERMS OF MATRICES

In this section, we show that a solution for Eq. (25) that defines the $s(\mathscr{C})$ can be found by using a matrix formulation that extends the technique used to compute the stationary weights $p(\mathscr{C})$. Its general solution is of the following form:

$$s(\mathscr{C}) = -\frac{1}{Z_N} \langle W| \prod_{i=1}^{N} (\tau_i X + (1-\tau_i) Y) |V\rangle + \text{const} \tag{32}$$

with $\tau_i = 1$ if site i is occupied and $\tau_i = 0$ if site i is empty, Z_N is given by (3), and the constant is arbitrary. The matrices X and Y and the vectors $\langle W|$ and $|V\rangle$ are given by

$$X = \begin{pmatrix} C & 0 & 0 & 0 & \cdot & \cdot \\ D & E & 0 & 0 & & \\ 0 & D & E & 0 & & \\ 0 & 0 & D & E & & \\ \cdot & & & \cdot & \cdot & \\ \cdot & & & & \cdot & \cdot \end{pmatrix} \quad \text{and} \quad Y = \begin{pmatrix} C & 0 & 0 & 0 & \cdot & \cdot \\ 0 & D & E & 0 & & \\ 0 & 0 & D & E & & \\ 0 & 0 & 0 & D & \cdot & \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & & \cdot \end{pmatrix} \tag{33}$$

$$\langle W| = (0, \langle\alpha|, \langle\alpha|, \langle\alpha| \quad \cdot \quad \cdot) \quad \text{and} \quad |V\rangle = \begin{pmatrix} |\beta\rangle \\ 0 \\ 0 \\ \cdot \\ \cdot \end{pmatrix} \tag{34}$$

where the matrices D, E, and C and the vectors $\langle\alpha|$ and $|\beta\rangle$ satisfy the algebraic rules (2).

Here X and Y are infinite-size matrices whose elements are themselves the infinite matrices D, E, and C. The $\langle W|$ and $|V\rangle$ are vectors whose components are themselves vectors. X and Y can be seen as operators on a tensor product of two infinite-dimensional spaces; $\langle W|$ and $|V\rangle$ are particular elements of this tensor product space. The structure of the $s(\mathscr{C})$ is more complicated than that of $p(\mathscr{C})$. This complexity is also apparent in the algebra generated by X, Y, $\langle W|$, and $|V\rangle$ (see Appendix B).

The proof that the $s(\mathscr{C})$ given by (32) do solve the linear equation (25) will use the following properties of the matrices X and Y and of the vectors $\langle W|$ and $|V\rangle$ (which are derived in Appendix B):

1. For all $p \geqslant 1$ and $q \geqslant 1$

$$XY^{p-1}(XY - YX) Y^{q-1}X = X^pY^qX + YX^pY^q - YX^{p-1}Y^qX - YX^pY^{q-1}X \tag{35}$$

2. For all $p \geqslant 1$ and $q \geqslant 1$

$$YX^{p-1}(XY-YX)\,Y^{q-1}\,|V\rangle = (X-Y)\,X^{p-1}Y^{q}\,|V\rangle \tag{36}$$

3. For all $p \geqslant 1$

$$\beta YX^{p-1}(X-Y)\,|V\rangle = (X-Y)\,X^{p-1}\,|V\rangle \tag{37}$$

4. For all $p \geqslant 1$ and $q \geqslant 1$

$$\langle W|\,X^{p-1}(XY-YX)\,Y^{q-1}X = \langle W|\,X^{p}Y^{q-1}(Y-X) + (\langle\alpha|\,C^{p+q}, 0, 0,...) \tag{38}$$

5. For all $p \geqslant 1$

$$\alpha\langle W|\,(Y-X)\,Y^{p-1}X = \langle W|\,Y^{p-1}(Y-X) + (\langle\alpha|\,C^{p} - \alpha\langle\alpha|\,C^{p+1}, 0, 0,...) \tag{39}$$

6. For a vector of the form $(\langle v|, 0, 0,...)$

$$(\langle v|, 0, 0,...)\,Y = (\langle v|, 0, 0,...)\,X = (\langle v|\,C, 0, 0,...) \tag{40}$$

and this is trivial when one looks at the matrices.

The first relation (35) of this algebra relates the system of size N with the system of size $N-1$, as each term in the r.h.s. contains one factor less than the terms in the l.h.s. This property plays a role similar to the equation $DE = D + E$ in (2). All the other properties are related to boundary effects.

To prove that the expression (32) of $s(\mathscr{C})$ solves Eq. (25), we shall write down explicitly the four different cases that can occur for simple types of configurations. A general proof for an arbitrary long configuration would follow exactly the same lines: all the terms arising from the displacement of a particle in the bulk of the lattice cancel out due to the first property (35), and there are only boundary terms left (i.e., a particle moving at the boundaries of the system). From these boundary terms, the properties (36)–(40) generate the r.h.s. of (25), by following exactly one of the four cases described below.

We use here a more convenient notation: a configuration starting by p occupied sites, followed by q empty sites, then r occupied sites, and ending with t empty sites is denoted by $1^p0^q1^r0^t$.

1. For a configuration of the form $1^p0^q1^r0^t$ with $p+q+r+t=N$, one can show from (36), (38), and (40) that

$$-2s(1^p0^q1^r0^t)+s(1^{p-1}010^{q-1}1^r0^t)+s(1^p0^q1^{r-1}010^{t-1})$$
$$=\frac{1}{Z_N}[\langle W| X^pY^qX^{r-1}(XY^t-YXY^{t-1})|V\rangle$$
$$+\langle W| X^{p-1}(XY-YX)\,Y^{q-1}X^rY^t|V\rangle]$$
$$=\frac{1}{Z_N}[\langle W| X^pY^{q-1}(X-Y)\,X^{r-1}Y^t|V\rangle$$
$$+\langle W| X^pY^{q-1}(Y-X)\,X^{r-1}Y^t|V\rangle$$
$$+(\langle\alpha| C^{p+q},0,0,...)\,X^{r-1}Y^t|V\rangle]$$
$$=\frac{1}{Z_N}\langle\alpha| C^{N-1}|\beta\rangle=J$$

2. For a configuration of the form $1^p0^q1^r$ with $p+q+r=N$, one can show from (37), (38), and (40) that

$$-(1+\beta)\,s(1^p0^q1^r)+s(1^{p-1}010^{q-1}1^r)+\beta s(1^p0^q1^{r-1}0)=J$$

3. For a configuration of the form $0^p1^q0^r$ with $p+q+r=N$, one can show from (36) and (39) that

$$-(\alpha+1)\,s(0^p1^q0^r)+\alpha s(10^{p-1}1^q0^r)+s(0^p1^{q-1}010^{r-1})=J-\alpha$$

4. For a configuration of the form $0^p1^q0^r1^t$ with $p+q+r+t=N$, one can show from (35), (37), (39), and (40) that

$$-(\alpha+1+\beta)\,s(0^p1^q0^r1^t)+\alpha s(10^{p-1}1^q0^r1^t)$$
$$+s(0^p1^{q-1}010^{r-1}1^t)+\beta s(0^p1^q0^r1^{t-1}0)=J-\alpha$$

4. EXPRESSIONS OF THE DIFFUSION CONSTANT

The diffusion constant Δ can now be rexpressed exactly as a sum of matrix elements, as it is just a linear combination (24) of the $s(\mathscr{C})$. In principle, analytical calculations are possible, but due to the complexity of the algebra (35)–(39) presented in the previous section, we could obtain simple closed expressions for Δ only in some particular cases ($\alpha=\beta=1$ and $\alpha+\beta=1$).

However, with the help of the matrices, a significant reduction of the numerical calculation times has occurred: instead of times growing exponentially with the system size, the matrices provide an algorithm whose time increases algebraically with size.

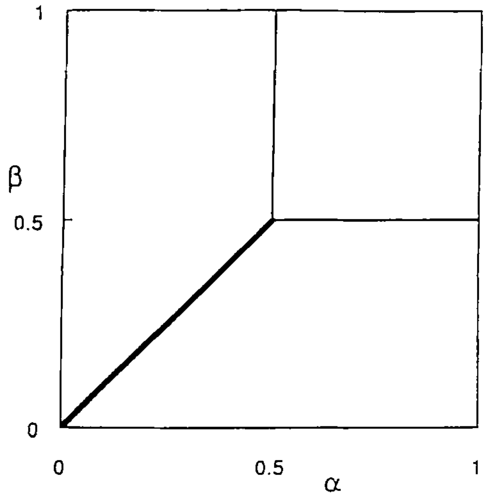

Fig. 1. The phase diagram of the model in the α–β plane. The region $\alpha > 1/2$ and $\beta > 1/2$ is the maximal current phase, whereas the region $\alpha < 1/2$ and $\beta > \alpha$ is the low-density phase and the region $\beta < 1/2$ and $\alpha > \beta$ is the high-density phase. The line $\alpha = \beta < 1/2$ is a first-order transition line.

When the size of the lattice goes to infinity, the system can undergo phase transitions on changing[2],[13–16] the values of α and β. The phase diagram consists of three phases (see Fig. 1):

- For $\alpha \geqslant 1/2$ and $\beta \geqslant 1/2$ the system is in the maximal current phase: the current and the mean occupation of a site do not depend on α, β and take values $J = 1/4$ and $\rho = 1/2$, respectively.
- For $\alpha < 1/2$ and $\beta > \alpha$ the system is in the low-density phase: $J = \alpha(1-\alpha)$ and $\rho = \alpha$.
- For $\beta < 1/2$ and $\beta < \alpha$ the system is in the high-density phase: $J = \beta(1-\beta)$ and $\rho = 1-\beta$.

Along the first-order transition line ($\alpha = \beta < 1/2$), the density profile is not constant in space, but increases linearly from α on the left to $1-\alpha$ on the right. Actually, this is an average over states of the system that exhibit a microscopic shock (a sharp discontinuity in the density profile) situated at an arbitrary position.[24]

Remark 3. It should be noticed that Δ is a symmetric function of α and β. In the ASEP, particles and holes play identical roles: holes are injected at the right-hand side rate β, and they move with hard-core exclusion toward the left, where they exit with rate α. The number Y_t of

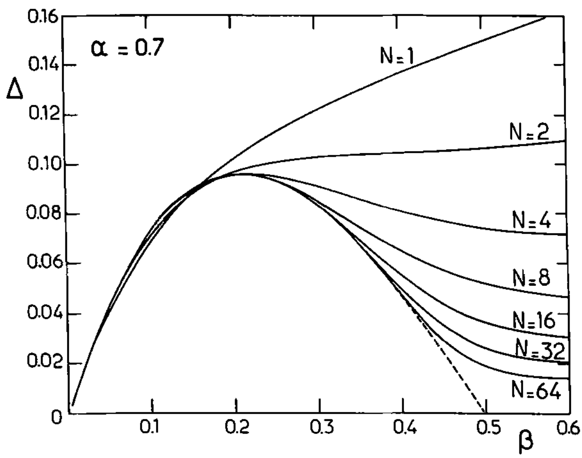

Fig. 2. The diffusion constant Δ versus β at fixed $\alpha = 0.7$ for various system sizes. The dashed line represents the limit $N \to \infty$ given by $\Delta = \beta(1-\beta)\,|1-2\beta|$ for $\beta < 1/2$. For $\beta > 1/2$, Δ vanishes in the thermodynamic limit.

particles entering the system is also the number of holes leaving it. The fluctuations of Y_t are identical to the fluctuations of the number of holes entering the system. Hence $\Delta(\alpha, \beta) = \Delta(\beta, \alpha)$.

4.1. Numerical Results

Some typical curves of Δ for many values of N and their limit as N goes to infinity are shown in Fig. 2–4. In each phase the limiting behavior of Δ can be deduced (in Section 4.3 we shall derive some of these expressions):

- For $\alpha \geqslant 1/2$ and $\beta \geqslant 1/2$, one sees that $\lim_{N \to \infty} \Delta = 0$. We shall show below that Δ is $\mathcal{O}(N^{-1/2})$.
- For $\alpha < 1/2$ and $\beta > \alpha$, $\Delta \to \alpha(1-\alpha)(1-2\alpha)$, when $N \to \infty$.
- For $\beta < 1/2$ and $\beta < \alpha$, by symmetry, $\Delta \to \beta(1-\beta)(1-2\beta)$, when $N \to \infty$.

When crossing the line $\alpha = \beta < 1/2$, one observes from Fig. 3 that the value of Δ changes rapidly. For N going to infinity, this behavior becomes a discontinuity in the graph of Δ. Numerically, the diffusion constant seems to fall to 2/3 of its value, i.e.,

$$\Delta(\alpha = \beta < \tfrac{1}{2}) = \tfrac{2}{3}\alpha(1-\alpha)(1-2\alpha) \tag{41}$$

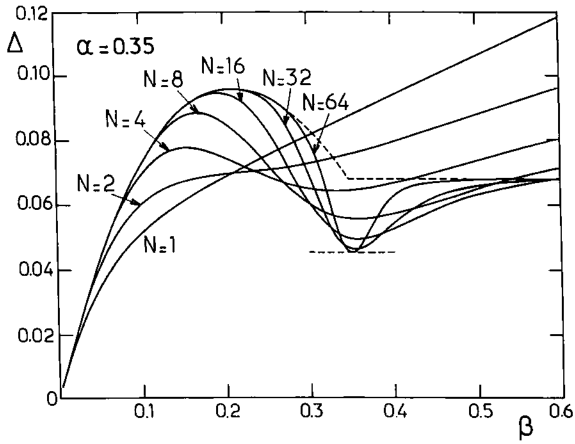

Fig. 3. The diffusion constant Δ versus β at fixed $\alpha = 0.35$. The results converge to $\Delta = \beta(1-\beta)\,|1-2\beta|$ for $\beta < \alpha$ and $\Delta = \alpha(1-\alpha)\,|1-2\alpha|$ for $\beta > \alpha$ (dashed curve) except along the first-order transition line $\alpha = \beta$, where $\Delta = \frac{2}{3}\beta(1-\beta)\,|1-2\beta|$ (represented by the horizontal line segment).

In the maximal current phase the asymptotic recovers the fact that for an infinite system the behavior is subdiffusive (i.e., Δ vanishes). The $\mathcal{O}(N^{-1/2})$ behavior is consistent with the $z = 3/2$ dynamical exponent in the KPZ equation in $(1+1)$ dimension.[22,25] On the other hand, in the high-density and low-density phases the (finite) asymptotic value of Δ is equal to the value obtained directly on an infinite system with a given density of particles.[21,26]

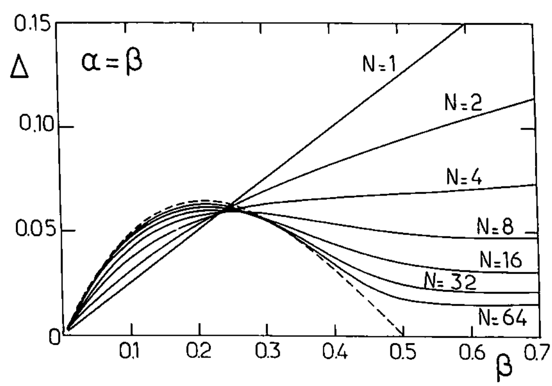

Fig. 4. Δ versus β along the first-order transition line $\alpha = \beta$. The results converge for $N \to \infty$ to the dashed curve $\Delta = \frac{2}{3}\beta(1-\beta)\,|1-2\beta|$ for $\beta < 1/2$ and to 0 for $\beta > 1/2$.

The factor 2/3 that appears in (41) on the line $\alpha = \beta < 1/2$ can be understood from the following simplified model: consider the situation where α $(=\beta)$ tends to zero $(\alpha \ll 1/N)$; in such a case the only configurations that have a nonnegligible probability of appearing are of the type 0000...0011111...11, i.e., a shock between a region of low density and a region of high density. Very occasionally a particle enters the system and after this happens the particle proceeds toward the position of the shock. The shock, on the arrival of the particle, moves one step to the left. Similarly, after a particle has been removed from the system, the shock moves one step to the right. Thus, counting the number of particles that enter the system is equivalent to counting the number of steps made toward the left by a random walker (who is situated at the position of the shock). This random walker moves to the right with probability $\alpha\, dt$ and to the left with probability $\alpha\, dt$ and there are reflecting boundaries at sites 0 and $N+1$. The solution of this random walk problem can be obtained by applying the formalism developed in Section 2. Here we only have N configurations $\mathscr{C}$ labeled by n, the position of the random walker. The equations for $p(\mathscr{C})$, (13), and $s(\mathscr{C})$, (25), can easily be solved to give $p(\mathscr{C}) = 1/N$, $s(\mathscr{C}) = n - n(n-1)/(2N)$. Equation (24) leads to

$$\Delta = \frac{\alpha(N-1)(2N-1)}{3N^2} \to \frac{2\alpha}{3}$$

This problem is fully equivalent to the problem of two particles on a ring which was solved in ref. 22 and the factor 2/3 already obtained.

For general $\alpha = \beta < 1/2$, if one assumes that the shock performs a random walk with probability $\mathscr{D}/2\, dt$ of moving to the right and probability $\mathscr{D}/2\, dt$ of moving to the left and if we relate Y_t to the number of left steps performed by the shock, denoted by x, multiplied by the difference between the densities to the right of the shock and to the left of shock, i.e., $Y_t = (1-2\alpha)x$, then

$$\langle Y_t^2 \rangle - \langle Y_t \rangle^2 = (1-2\alpha)^2 [\langle x^2 \rangle - \langle x \rangle^2] \tag{42}$$

As before, due to the reflecting boundaries, $\langle x^2 \rangle - \langle x \rangle^2$ is given by $(2/3)(\mathscr{D}/2)\, t$, so that

$$\langle Y_t^2 \rangle - \langle Y_t \rangle^2 \to (1-2\alpha)^2\, \tfrac{1}{3} \mathscr{D} t \tag{43}$$

Our result (1) would then imply

$$\mathscr{D} = \frac{2\alpha(1-\alpha)}{1-2\alpha} \tag{44}$$

This is consistent with a recent work of Ferrari and Fontes,[27] who proved that in an infinite system with no boundaries the motion of a shock converges in distribution to Brownian motion with diffusion constant $\mathscr{D}$ given in the present case of densities α to the left and $1-\alpha$ to the right by (44).

Krug and Tang[28] recently reinterpreted the exact results for the ASEP with open boundaries in terms of a directed polymer in a random medium confined between two walls. The current in the ASEP measures the mean energy per unit length of a directed polymer of infinite length and the diffusion constant measures the variance of the energy per unit length. The low- and high-density phases correspond to bound states of the polymer at the walls, whereas the maximal current phase corresponds to a polymer free to move. Since in the bound state the directed polymer experiences a one-dimensional disorder, it is not surprising to find in that case a nonzero diffusion constant.

4.2. Exact Expressions for Δ

The diffusion constant Δ can be expressed in terms of matrix elements, by substituting in (24) the expression of the $s(\mathscr{C})$. We could explicitly perform this sum in two particular cases, $\alpha=1$ and $\alpha+\beta=1$, which we describe below. The exact formulas obtained will enable us to confirm the asymptotic behavior of Δ in the limit of infinite lattice size in each region of the phase diagram and to support the conclusions drawn from the numerical data.

In order to derive an explicit expression for the diffusion constant one has to consider the following sums [see (24)]:

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \sum_{\{\tau_i=1,0;\,1\leqslant i\leqslant N\}} \langle\alpha| \left[\prod_{i=1}^{N} \tau_i D+(1-\tau_i)\, E\right] |\beta\rangle \times \langle W| \left[\prod_{i=1}^{N} \tau_i X+(1-\tau_i)\, Y\right] |V\rangle \tag{45}$$

$$\sum_{\mathscr{C},\mathscr{C}'} M_1(\mathscr{C},\mathscr{C}')\, p(\mathscr{C}')\, s(\mathscr{C}) = -\frac{\alpha}{Z_N^2} \sum_{\{\tau_i=1,0;\,2\leqslant i\leqslant N\}} \langle\alpha|\, E\left[\prod_{i=2}^{N} \tau_i D+(1-\tau_i) E\right] |\beta\rangle \times \langle W|\, X\left[\prod_{i=2}^{N} \tau_i X+(1-\tau_i)\, Y\right] |V\rangle \tag{46}$$

If one introduces G given by

$$G = D \otimes X + E \otimes Y \tag{47}$$

where the notation $A \otimes B$ simply means the matrix A with each of its elements replaced by the original element multiplied by matrix B, then the quantities (45) and (46) may be written as

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \langle \alpha | \otimes \langle W |\, G^N \,| \beta \rangle \otimes | V \rangle \tag{48}$$

$$\sum_{\mathscr{C}, \mathscr{C}'} M_1(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}')\, s(\mathscr{C}) = -\frac{1}{Z_N^2} [\langle \alpha | \otimes \langle W |\, X]\, G^{N-1} \,| \beta \rangle \otimes | V \rangle \tag{49}$$

Again the notation $\langle a | \otimes \langle b |$ simply means the vector $\langle a |$ with each of its elements replaced by the original element multiplied by vector $\langle b |$. Thus the computation of the diffusion constant amounts to calculating certain elements (48) and (49) of powers of G, which may be considered as a matrix whose elements are matrices whose elements are matrices. In Appendix C we show how explicit expressions for such matrix elements may be calculated in two cases, $\alpha = \beta = 1$ and $\alpha + \beta = 1$. Let us state here the results.

- For $\alpha + \beta = 1$

$$\Delta = J \left(1 - 2J \sum_{k=0}^{N-1} \frac{(2k)!}{k!\,(k+1)!} J^k \right) \tag{50}$$

where $J = \alpha(1 - \alpha)$.

- For $\alpha = 1$, $\beta = 1$

$$\Delta = \frac{3(4N+1)!\,[N!\,(N+2)!]^2}{2[(2N+1)!]^3 (2N+3)!} \tag{51}$$

4.3. Asymptotic Limits of Exact Expressions

Here we shall deduce the asymptotic limits of Δ in the various phases by considering the specific cases where we obtained exact expressions for the diffusion constant:

- For $\alpha + \beta = 1$, $\alpha \neq \beta$

$$\Delta \to \beta(1 - \beta)\, |1 - 2\beta| \tag{52}$$

- For $\alpha+\beta=1$, $\alpha=\beta=1/2$

$$\Delta \simeq \frac{1}{4\pi^{1/2}N^{1/2}} \tag{53}$$

- For $\alpha=1$, $\beta=1$

$$\Delta \simeq \frac{3(2\pi)^{1/2}}{64N^{1/2}} \tag{54}$$

Expressions (52) and (53) are the asymptotics along the line of parameter values where the steady state factorizes. This line traverses both the high-density and low-density phases, in which case (52) is the asymptotic, and also the point in the phase diagram where the maximal current phase joins the high-density and low-density phases, in which case (53) is the asymptotic. Both (52) and (53) are consistent with our numerical results. They can be obtained by using the asymptotic forms of the sum involved in (50).

For $J<1/4$

$$\sum_{k=0}^{N-1} \frac{(2k)!}{k!\,(k+1)!} J^k = \frac{1-(1-4J)^{1/2}}{2J} - \frac{(4J)^N}{\pi^{1/2}N^{3/2}} \frac{1}{1-4J} + \cdots \tag{55}$$

For $J=1/4$

$$\sum_{k=0}^{N-1} \frac{(2k)!}{k!\,(k+1)!} J^k = 2 - \frac{2}{\pi^{1/2}N^{1/2}} + \frac{1}{4\pi^{1/2}N^{3/2}} + \cdots \tag{56}$$

Expression (54) is for one point within the maximal current phase and is easy to obtain from (51) by using Stirling's formula.

We see from (53)–(54) that in and on the boundaries of the high-density phase the diffusion constant is $\mathcal{O}(N^{-1/2})$. In principle the general formula (58) to be given below should allow one to check this fact and to calculate the prefactor of $N^{-1/2}$ in the whole of the maximal current phase.

Remark 4. For general values of α and β we find that

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C})$$

$$= -\sum_{n=1}^{N} \frac{\langle\alpha|\, C^{n-1}DC^{N-n}\,|\beta\rangle}{\langle\alpha|\, C^N\,|\beta\rangle} + \sum_{n=0}^{N-1} (N-n) \frac{(2n)!}{n!\,(n+1)!} \frac{\langle\alpha|\, C^{N-n-1}\,|\beta\rangle}{\langle\alpha|\, C^N\,|\beta\rangle}$$

$$-\sum_{n=1}^{N} \frac{\langle\alpha|\, C^{N-n}\,|\beta\rangle}{\langle\alpha|\, C^N\,|\beta\rangle^2} [\langle\alpha|\, C^{n-1}DC^N\,|\beta\rangle - \langle\alpha|\, C^N DC^{n-1}\,|\beta\rangle \tag{57}$$

and

$$\Delta = \frac{\langle\alpha|\, C^{N-1}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle} - \frac{\langle\alpha|\, C^{N-1}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle} \sum_{n=1}^{N-1} \left[\frac{\langle\alpha|\, C^{n-1} D C^{N-n}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle} - \frac{\langle\alpha|\, C^{n-1} D C^{N-1-n}\,|\beta\rangle}{\langle\alpha|\, C^{N-1}\,|\beta\rangle} \right]$$
$$+ \sum_{n=0}^{N-1} \frac{(2n)!}{n!\,(n+1)!} \left[(N-n-1)\, \frac{\langle\alpha|\, C^{N-n-2}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle} - (N-n+1)\, \frac{\langle\alpha|\, C^{N-1}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle} \frac{\langle\alpha|\, C^{N-n-1}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle} \right]$$
$$+ 2\, \frac{\langle\alpha|\, C^{N-1}\,|\beta\rangle}{\langle\alpha|\, C^{N}\,|\beta\rangle^{3}} \sum_{n=1}^{N} \langle\alpha|\, C^{N-n}\,|\beta\rangle \times [\langle\alpha|\, C^{n-1} D C^{N}\,|\beta\rangle - \langle\alpha|\, C^{N} D C^{n-1}\,|\beta\rangle]$$
$$- \frac{1}{\langle\alpha|\, C^{N}\,|\beta\rangle^{2}} \sum_{n=1}^{N-1} \langle\alpha|\, C^{N-n}\,|\beta\rangle \times [\langle\alpha|\, C^{n-1} D C^{N-1}\,|\beta\rangle - \langle\alpha|\, C^{N-1} D C^{n-1}\,|\beta\rangle]$$
$$- \frac{1}{\langle\alpha|\, C^{N}\,|\beta\rangle^{2}} \sum_{n=1}^{N-1} \langle\alpha|\, C^{N-n-1}\,|\beta\rangle \times [\langle\alpha|\, C^{n-1} D C^{N}\,|\beta\rangle - \langle\alpha|\, C^{N-1} D C^{n}\,|\beta\rangle] \tag{58}$$

where the matrix elements involved are given by expressions derived in ref. 14:

$$\langle\alpha|\, C^{N}\,|\beta\rangle = \frac{\alpha\beta}{\alpha-\beta} \left[R_N\left(\frac{1}{\beta}\right) - R_N\left(\frac{1}{\alpha}\right) \right] \langle\alpha \mid \beta\rangle \tag{59}$$

$$\langle\alpha|\, C^{m} D C^{n}\,|\beta\rangle = \sum_{p=0}^{n-1} \frac{(2p)!}{p!\,(p+1)!} \langle\alpha|\, C^{n+m-p}\,|\beta\rangle + R_n\left(\frac{1}{\beta}\right) \langle\alpha|\, C^{m}\,|\beta\rangle \tag{60}$$

where

$$R_n\left(\frac{1}{\beta}\right) = \sum_{p=1}^{n} \frac{p(2n-1-p)!}{n!\,(n-p)!} \frac{1}{\beta^{p+1}} \qquad \text{for} \quad n \geqslant 1$$
$$R_0\left(\frac{1}{\beta}\right) = \frac{1}{\beta} \tag{61}$$

The expressions (57) and (58) can be obtained using ideas similar to those employed in the proof for the case $\alpha=\beta=1$, outlined in Appendix C. However, the derivation for the general case is far more complicated and we do not feel that it would at all be instructive to present it here. We checked (57) and (58) on the computer for a number of choices of α, β, and N and they were in perfect agreement with a direct numerical calculation of the two sums (45) and (46).

5. RELATION WITH CORRELATION FUNCTIONS

In this section, we explain how the quantities $s(\mathscr{C})$ and Δ are related to some non-equal-time correlation functions of the ASEP. This will shed some light on the physical meaning of the $s(\mathscr{C})$, and show that matrix techniques can be useful in calculating more general properties than equal-time correlation functions.

Between times t and $t+dt$, the number Y_t of particles which have entered the system since $t=0$ increases by one unit with probability $\alpha\, dt$ if the first site of the lattice is empty. If one decomposes the time interval $[0, t]$ into t/dt infinitesimal intervals of duration dt, Y_t can be written as

$$Y_t = \sum_{k=1}^{t/dt} a_k \tag{62}$$

where a_k is a random variable that takes two values, 0 or 1: $a_k=1$ if a particle has entered the system in the kth small time interval dt {this occurs with probability $\alpha[1-\tau_1(k\, dt)]\, dt$}; $a_k=0$ if no particle has entered in the time interval {this occurs with probability $1-\alpha[1-\tau_1(k\, dt)]\, dt$}.

One can then derive some new expressions for $\langle Y_t \mid \mathscr{C}_0\rangle$, the average of Y_t starting from a specific configuration $\mathscr{C}_0$, and for $\langle Y_t\rangle^2$ [when the initial configuration is not specified, it means that an average is taken over the initial configurations with their stationary weights $p(\mathscr{C})$]. Taking averages of (62) and going to the continuous limit, one obtains

$$\begin{aligned}\langle Y_t \mid \mathscr{C}_0\rangle &= \sum_{k=1}^{t/dt} \langle a_k \mid \mathscr{C}_0\rangle = \sum_{k=1}^{t/dt} \alpha\langle [1-\tau_1(k dt)] \mid \mathscr{C}_0\rangle\, dt \\ &= \alpha \int_0^t [1-\langle \tau_1(t') \mid \mathscr{C}_0\rangle]\, dt' \end{aligned}\tag{63}$$

The system reaches a steady-state when time goes to infinity, so

$$\langle \tau_1(t) \mid \mathscr{C}_0\rangle \to \langle \tau_1\rangle \tag{64}$$

where $\langle \tau_1 \rangle$ is the probability of the first site being occupied in the stationary state. Formula (63) can then be rewritten as

$$\langle Y_t \mid \mathscr{C}_0 \rangle = \alpha(1 - \langle \tau_1 \rangle) t + \alpha \int_0^t [\langle \tau_1 \rangle - \langle \tau_1(t') \mid \mathscr{C}_0 \rangle] \, dt' \tag{65}$$

From Section 1, we know that the asymptotic behavior of $\langle Y_t \mid \mathscr{C}_0 \rangle$ can also be deduced from that of $q_t(\mathscr{C} \mid \mathscr{C}_0)$ just by summing (18) over $\mathscr{C}$:

$$\langle Y_t \mid \mathscr{C}_0 \rangle - Jt \to s(\mathscr{C}_0) + \sum_{\mathscr{C}} r(\mathscr{C}) \tag{66}$$

If one averages (66) with respect to the stationary probabilities $p(\mathscr{C}_0)$ and uses the fact (8) that $\langle Y_t \rangle = Jt$, one obtains the following relation between the quantities $s(\mathscr{C}_0)$ and $r(\mathscr{C})$:

$$\sum_{\mathscr{C}} r(\mathscr{C}) + \sum_{\mathscr{C}_0} s(\mathscr{C}_0) \, p(\mathscr{C}_0) = 0 \tag{67}$$

One can then rewrite (66) in the following form, which uses only the quantities $s(\mathscr{C}_0)$:

$$\langle Y_t \mid \mathscr{C}_0 \rangle - Jt \to s(\mathscr{C}_0) - \sum_{\mathscr{C}} s(\mathscr{C}) \, p(\mathscr{C}) \tag{68}$$

Comparison of (65) with (68) provides an integral expression for $s(\mathscr{C}_0)$:

$$\alpha \int_0^\infty [\langle \tau_1 \rangle - \langle \tau_1(t) \mid \mathscr{C}_0 \rangle] \, dt = s(\mathscr{C}_0) - \sum_{\mathscr{C}} s(\mathscr{C}) \, p(\mathscr{C}) \tag{69}$$

The left-hand side of this equation represents the time integral of a non-equal-time correlation function and we have shown that for any initial configuration $\mathscr{C}_0$, the right-hand side can be written as matrix elements. Roughly speaking, one can say that the quantities $s(\mathscr{C}_0)$ measure the relaxation of the current to its equilibrium value.

One can derive an expression for the fluctuations of Y_t in a similar fashion, by using the same discretization as before (2). Briefly, one has

$$\begin{aligned}
&\langle Y_t^2 \rangle - \langle Y_t \rangle^2 \\
&= \left\langle \left(\sum_{k=1}^{t/dt} a_k \right)^2 \right\rangle - \left(\sum_{k=1}^{t/dt} \langle a_k \rangle \right)^2 \\
&= \sum_{k=1}^{t/dt} (\langle a_k^2 \rangle - \langle a_k \rangle^2) + 2 \sum_k \sum_{j<k} \langle a_k a_j \rangle - \langle a_k \rangle \langle a_j \rangle
\end{aligned}$$

$$= \alpha \int_0^t dt' \langle 1 - \tau_1(t') \rangle + 2\alpha^2 \int_0^t dt' \int_0^{t'} dt'' \langle [1 - \tau_1(t'')][1 - \tau_1(t')] \rangle - \langle 1 - \tau_1(t'') \rangle \langle 1 - \tau_1(t') \rangle$$

$$= \alpha \int_0^t \langle 1 - \tau_1(t') \rangle \, dt' + 2\alpha^2 \int_0^t dt' \int_0^{t'} dt'' \langle \tau_1(t'') \, \tau_1(0) \rangle - \langle \tau_1(t'') \rangle \langle \tau_1(0) \rangle \tag{70}$$

where we have used the time translation invariance of the correlation functions. The expression of Δ in terms of non-equal-time correlation functions is finally deduced:

$$\Delta = \lim_{t \to \infty} \frac{\langle Y_t^2 \rangle - \langle Y_t \rangle^2}{t}$$

$$= J + 2\alpha^2 \int_0^\infty [\langle \tau_1(t) \, \tau_1(0) \rangle - \langle \tau_1 \rangle^2] \, dt \tag{71}$$

Remark 5. Instead of counting the number Y_t of particles that have entered the system since $t = 0$, we could have marked the ith bond of the lattice (between sites i and $i + 1$) and looked at $Y_t^{(i)}$ ($i = 1,..., N - 1$), the number of particles that have passed through that bond during time t. We could also have studied $Y_t^{(N)}$, the number of particles having left the system during time t.

The reasoning is readily modified for each case: the transition matrix M has to be split into two parts M_0 and M_1: but now $M_0(\mathscr{C}_1, \mathscr{C}_0) \, dt$ is the probability of going from $\mathscr{C}_0$ to $\mathscr{C}_1$ without a particle passing through bond i and $M_1(\mathscr{C}_1, \mathscr{C}_0) \, dt$ is the probability of going from $\mathscr{C}_0$ to $\mathscr{C}_1$ by a particle passing through bond i, in a time interval dt.

At any time all the $Y_t^{(i)}$ differ by an integer less than N. Their fluctuations thus have the same rate of growth with time: the diffusion constant computed for any $Y_t^{(i)}$ is identical to Δ.

All the relations of this section derived for Y will remain true for $Y^{(i)}$ once the expression $\alpha[1 - \tau_1(t)]$ is replaced by $\tau_i(t)[1 - \tau_{i+1}(t)]$, for $i = 1,..., N - 1$, and by $\beta \tau_N(t)$ for $Y_t^{(N)}$. For instance, we obtain the following formulas for Δ:

$$\Delta = J + 2 \int_0^\infty dt \, \langle \tau_i(t)[1 - \tau_{i+1}(t)][1 - \tau_{i+1}(0)] \, \tau_i(0) \rangle - \langle [1 - \tau_{i+1}] \tau_i \rangle^2$$

$$= J + 2\beta^2 \int_0^\infty \langle \tau_N(t) \, \tau_N(0) \rangle - \langle \tau_N \rangle^2$$

For each i, the functions $s_i(\mathscr{C})$ are defined as in Section 1 and they are solutions of the same inhomogeneous equation as (25), but with the relevant M_1 (as described above)

$$\sum_{\mathscr{C}_1} s_i(\mathscr{C}_1)\, M(\mathscr{C}_1, \mathscr{C}_0) = J - \sum_{\mathscr{C}_1} M_1(\mathscr{C}_1, \mathscr{C}_0)$$

A solution of this equation is found by setting

$$s_i(\mathscr{C}) = s(\mathscr{C}) + n_i(\mathscr{C})$$

where $n(\mathscr{C})$ is the number of occupied sites in configuration $\mathscr{C}$ between site 1 and site i (inclusive). Thus our approach should allow one to compute correlation functions of the following type:

$$s_i(\mathscr{C}_0) - \sum_{\mathscr{C}} p(\mathscr{C})\, s_i(\mathscr{C}) = \int_0^\infty \langle \tau_i[1-\tau_{i+1}]\rangle - \langle \tau_i(t)[1-\tau_{i+1}(t)] \mid \mathscr{C}_0\rangle\, dt$$

6. CONCLUSION

In this paper we have shown that the fluctuations of the current through a bond of a finite system with open boundary conditions can be calculated exactly. Our approach required the solution of an inhomogeneous master Eq. (25).

We have shown that this inhomogeneous master equation can be solved using a generalization of the matrix approach which had been developed to describe the steady-state. As the generalization of the matrix approach to the present case is rather complicated, we have shown how to perform the last sum (24), which yields the diffusion constant, only in some particular cases, (50) and (51). For the general case we present (58) without proof.

Our result shows that the diffusion constant Δ is singular when one crosses the phase boundaries. In particular, along the first-order transition line, it is discontinuous with a drop to 2/3 of its value. Inside the low- and the high-density phases, its expression in the thermodynamic limit is in agreement with the recent results of Ferrari and Fontes.[21,27]

Our hope in calculating exactly this diffusion constant was to try and better understand the non-equal-time steady-state properties of the asymmetric exclusion model. Indeed, the diffusion constants calculated here and in ref. 22 can be thought of as the simplest non-equal-time steady-state quantities. Unfortunately, the solution we have obtained is too complicated to be generalized in its present form to calculate other non-equal-time steady-state properties. So perhaps to make further progress on the non-equal-time properties of the asymmetric exclusion model, it would first be better to look for a simpler derivation of the results obtained in the present work.

APPENDIX A

In this appendix we obtain the asymptotic behavior (17), (18) of $p_t(\mathscr{C} \mid \mathscr{C}_0)$ and $q_t(\mathscr{C} \mid \mathscr{C}_0)$. This gives explicit expressions of the $s(\mathscr{C})$ and $r(\mathscr{C})$ in terms of the eigenvectors and eigenvalues of M. For simplicity, we will assume that the matrix M is diagonalizable (the nondiagonalizable case can also be treated, but would require more complicated notation). The matrix $M(\mathscr{C}, \mathscr{C}')$ has 2^N eigenvalues $\lambda_1 ..., \lambda_{2^N}$, one of which is zero, with all the others less than 0,

$$\lambda_1 = 0 \qquad \text{and} \qquad \lambda_n < 0 \quad \text{for} \quad n \geqslant 2 \tag{A1}$$

Let us denote by χ_n and ψ_n the normalized right and left eigenvectors of the matrix $M(\mathscr{C}, \mathscr{C}')$:

$$\lambda_n \chi_n(\mathscr{C}) = \sum_{\mathscr{C}'} M(\mathscr{C}, \mathscr{C}')\, \chi_n(\mathscr{C}') \tag{A2}$$

$$\lambda_n \psi_n(\mathscr{C}') = \sum_{\mathscr{C}} \psi_n(\mathscr{C})\, M(\mathscr{C}, \mathscr{C}') \tag{A3}$$

These eigenvectors are normalized to have

$$\sum_{\mathscr{C}} \psi_n(\mathscr{C})\, \chi_{n'}(\mathscr{C}) = \delta_{n,n'} \tag{A4}$$

and they form a complete set so that

$$\sum_n \chi_n(\mathscr{C})\, \psi_n(\mathscr{C}') = \delta_{\mathscr{C},\mathscr{C}'} \tag{A5}$$

The equations (15) and (16) governing the evolution of $p_t(\mathscr{C} \mid \mathscr{C}_0)$ and $q_t(\mathscr{C} \mid \mathscr{C}_0)$ can formally be solved. One finds, by taking into account the initial condition $p_0(\mathscr{C} \mid \mathscr{C}_0) = \delta_{\mathscr{C},\mathscr{C}_0}$,

$$p_t(\mathscr{C} \mid \mathscr{C}_0) = e^{Mt}(\mathscr{C}, \mathscr{C}_0) \tag{A6}$$

Hence, by projecting on the eigenvectors, one obtains

$$p_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_n \chi_n(\mathscr{C})\, e^{\lambda_n t}\, \psi_n(\mathscr{C}_0) \tag{A7}$$

Similarly, after inserting $p_t = \exp Mt$ into (16) and taking into account the initial condition $q_0 = 0$, one has

$$q_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}'', \mathscr{C}'} \int_0^t d\tau\, p_\tau(\mathscr{C} \mid \mathscr{C}'')\, M_1(\mathscr{C}'', \mathscr{C}')\, p_{t-\tau}(\mathscr{C}' \mid \mathscr{C}_0) \tag{A8}$$

which can be rewritten as

$$q_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{\mathscr{C}'', \mathscr{C}'} \sum_{n, n'} \int_0^t d\tau\, \chi_n(\mathscr{C})\, e^{\lambda_n \tau} \psi_n(\mathscr{C}'')\, M_1(\mathscr{C}'', \mathscr{C}')\, \chi_{n'}(\mathscr{C}')\, e^{\lambda_{n'}(t-\tau)}\, \psi_{n'}(\mathscr{C}_0) \tag{A9}$$

If one defines

$$m_1(n, n') = \sum_{\mathscr{C}'', \mathscr{C}'} \psi_n(\mathscr{C}'')\, M_1(\mathscr{C}'', \mathscr{C}')\, \chi_{n'}(\mathscr{C}') \tag{A10}$$

one finds that

$$q_t(\mathscr{C} \mid \mathscr{C}_0) = \sum_{n, n'} \int_0^t d\tau\, \chi_n(\mathscr{C})\, e^{\lambda_n \tau} m_1(n, n')\, e^{\lambda_{n'}(t-\tau)} \psi_{n'}(\mathscr{C}_0) \tag{A11}$$

In the long-time limit, as all the λ_n but λ_1 are strictly negative, the expected asymptotic behavior is obtained:

$$p_t(\mathscr{C} \mid \mathscr{C}_0) \to \chi_1(\mathscr{C})\, \psi_1(\mathscr{C}_0) \tag{A12}$$

In expression (A11), the factor, $\int_0^t d\tau \exp(\lambda_{n'}\tau) \exp[\lambda_n(t-\tau)]$ goes exponentially to zero if both n and n' are different from 1; it goes to the constant $-1/\lambda_n$ if $n' = 1$ and to $-1/\lambda_{n'}$ if $n = 1$; it is equal to t if $n = n' = 1$. From this we deduce the asymptotic behavior:

$$\begin{aligned} q_t(\mathscr{C} \mid \mathscr{C}_0) \to {} & t\chi_1(\mathscr{C})\, m_1(1, 1)\, \psi_1(\mathscr{C}_0) - \chi_1(\mathscr{C}) \sum_{n' > 1} \frac{m_1(1, n')}{\lambda_{n'}} \psi_{n'}(\mathscr{C}_0) \\ & - \sum_{n > 1} \chi_n(\mathscr{C}) \frac{m_1(n, 1)}{\lambda_n} \psi_1(\mathscr{C}_0) \end{aligned} \tag{A13}$$

and we recover the expected asymptotic behavior (17), (18) by making the following identifications:

$$\chi_1(\mathscr{C}) = p(\mathscr{C}) \tag{A14}$$

$$\psi_1(\mathscr{C}_0) = 1 \tag{A15}$$

$$J = m_1(1, 1) \tag{A16}$$

$$r(C) = -\sum_{n>1} \chi_n(\mathscr{C}) \frac{m_1(n, 1)}{\lambda_n} \tag{A17}$$

$$s(\mathscr{C}_0) = -\sum_{n>1} \frac{m_1(1, n)}{\lambda_n} \psi_n(\mathscr{C}_0) \tag{A18}$$

Finally, by using (24), we may express Δ as

$$\Delta = m_1(1, 1) - 2 \sum_{n>1} \frac{m_1(1, n)\, m_1(n, 1)}{\lambda_n} \tag{A19}$$

APPENDIX B

In this appendix, we shall prove the algebraic properties (35)–(39) satisfied by the matrices X and Y and the vectors $\langle W|$ and $|V\rangle$. We use the notation

$$\langle 1| \langle v| \equiv (\langle v|, 0, 0, 0, \ldots)$$

Also, when we use a lowercase letter for an operator, it means that it acts on the second part of the vector. Thus, we have, for example,

$$\langle 1| \langle v| c = (\langle v| C, 0, 0, 0, \ldots) \tag{B1}$$

Equivalently, one can write

$$c = \begin{pmatrix} C & 0 & 0 & 0 & \cdot & \cdot \\ 0 & C & 0 & 0 & & \\ 0 & 0 & C & 0 & & \\ 0 & 0 & 0 & C & \cdot & \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & & \cdot \end{pmatrix} \tag{B2}$$

Preliminary Results

If one defines the operator ψ by

$$\psi = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & -1 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ 0 & 0 & 0 & 0 & & \\ \cdot & & & & & \cdot \\ \cdot & & & & & \cdot \end{pmatrix} \tag{B3}$$

It is easy to prove the following from (33):

1. We have

$$\psi^2 = -\psi \tag{B4}$$

2. We have

$$XY - YX = c\psi = \psi c = d\psi + \psi e = \psi d + e\psi \tag{B5}$$

3. We also have

$$\psi X = e\psi = \psi e \tag{B6}$$

$$Y\psi = d\psi = \psi d \tag{B7}$$

Relations (B4)–(B7) are direct consequences of the definition of ψ and of the fact that $C = DE = D + E$.

4. For all $p \geqslant 1$

$$XY^p - Y^pX = d\psi Y^{p-1}X \tag{B8}$$

$$X^pY - YX^p = YX^{p-1}\psi e \tag{B9}$$

Proof of (B8) and (B9): the case $p = 1$ of (B8)–(B9) is a simple consequence of (B5)–(B7) and of the fact that $de = c$. One can then prove (B8) by recursion: assume that it is true for $p - 1$

$$XY^{p-1} - Y^{p-1}X = d\psi Y^{p-2}X$$

Then one can write

$$\begin{aligned} XY^p - Y^pX &= (XY^{p-1} - Y^{p-1}X)\, Y + Y^{p-1}(XY - YX) \\ &= d\psi Y^{p-2}XY + Y^{p-1}c\psi \end{aligned}$$

This can be written, using (B5), as

$$XY^p - Y^pX = d\psi Y^{p-1}X + d\psi Y^{p-2}\psi c + Y^{p-1}\psi c$$

which reduces to (B8) when using (B4) and (B7). The proof of (B9) is almost identical: One writes

$$X^pY - YX^p = X(X^{p-1}Y - YX^{p-1}) + (XY - YX)\, X^{p-1}$$

Then, assuming that (B9) is true up to $p - 1$, one finds

$$X^pY - YX^p = XYX^{p-2}\psi e + c\psi X^{p-1} = YX^{p-1}\psi e$$

5. The action of Y on a vector of the form of $|W\rangle$ gives a vector of the same form, i.e.,

$$Y\begin{pmatrix} |v\rangle \\ 0 \\ 0 \\ \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} C\,|v\rangle \\ 0 \\ 0 \\ \cdot \\ \cdot \end{pmatrix} \tag{B10}$$

Moreover, from (33) and (B4), one can easily show that

$$0 = (X - Y - d\psi)\begin{pmatrix} |v\rangle \\ 0 \\ 0 \\ \cdot \\ \cdot \end{pmatrix} \tag{B11}$$

6. Similarly,

$$(\langle v|, \langle w|, \langle w|, \langle w|,...)X = (\langle v'|, \langle w|\; C, \langle w|\; C, \langle w|\; C,...)$$

and

$$(\langle v|, \langle w|, \langle w|, \langle w|,...)(X - Y + e\psi) = (\langle w|\; C, 0, 0,...) \tag{B12}$$

Proofs of (35)–(39)

Proof of (35). Using (B5), one has

$$YX^{p-1}(XY - YX)\; Y^{q-1}X = YX^{p-1}(d\psi + \psi e)\; Y^{q-1}X$$

Then the proof follows using (B8) and (B9).

Proof of (36). Using (B5), one obtains

$$YX^{p-1}(XY - YX)\; Y^{q-1}\,|V\rangle = YX^{p-1}(d\psi + \psi e)\; Y^{q-1}\,|V\rangle$$

Then, using (B9), one finds

$$\begin{aligned} &YX^{p-1}(XY - YX)\; Y^{q-1}\,|V\rangle \\ &\quad = [\,YX^{p-1}\,d\psi\, Y^{q-1} + X^pY^q - YX^pY^{q-1}]\,|V\rangle \end{aligned}$$

and the proof of (36) follows from (B10) and (B11), which imply that

$$YX^{p-1}[\,Y + d\psi - X]\; Y^{q-1}\,|V\rangle = 0$$

Proof of (37). The case $p=1$ is easy to check from (33), (34), and (2):

$$\beta Y(X-Y)\,|V\rangle = (X-Y)\,|V\rangle$$

Assuming that (37) is true up to $p-1$, let us now prove (37) for p. One has

$$\begin{aligned}
&\beta(YX^{p}-YX^{p-1}Y)\,|V\rangle \\
&\quad = \beta(YX-XY)(X^{p-1}-X^{p-2}Y)\,|V\rangle + X(X-Y)\,X^{p-2}\,|V\rangle
\end{aligned}$$

Then, using (B5), one obtains

$$\beta YX^{p-1}(X-Y)\,|V\rangle = -\beta c\psi(X^{p-1}-X^{p-2}Y)\,|V\rangle + (X^{p}-XYX^{p-2})\,|V\rangle$$

which after (B5) is applied again becomes

$$\beta YX^{p-1}(X-Y)\,|V\rangle = c\psi X^{p-2}(\beta(Y-X)-1)\,|V\rangle + (X^{p}-YX^{p-1})\,|V\rangle$$

which yields, using (B11) and (2),

$$\beta YX^{p-1}(X-Y)\,|V\rangle = c\psi X^{p-2}(-\psi-1)\,|V\rangle + (X^{p}-YX^{p-1})\,|V\rangle$$

The proof then follows from (B6) and (B4).

Proof of (38). Using (B5), one has

$$\langle W|\,X^{p-1}(XY-YX)\,Y^{q-1}X = \langle W|\,X^{p-1}(d\psi+e\psi)\,Y^{q-1}X$$

Then, using (B8), one finds

$$\begin{aligned}
&\langle W|\,X^{p-1}(XY-YX)\,Y^{q-1}X \\
&\quad = \langle W|\,X^{p-1}(XY^{q}-Y^{q}X+e\psi Y^{q-1}X) \\
&\quad = \langle W|\,[X^{p}Y^{q-1}(Y-X)+X^{p-1}(X-Y+e\psi)\,Y^{q-1}X]
\end{aligned}$$

which, using (B12) and (40), gives the proof of (38).

Proof of (39). Let us start with $p=1$. Using (B12), one has

$$\alpha\langle W|\,(Y-X)X = \alpha\langle W|\,e\psi X - \alpha(\langle\alpha|\,C^{2},0,0,\ldots)$$

which, using (B6), (2), and (33), becomes

$$\alpha\langle W|\,(Y-X)X = \langle W|\,e\psi - \alpha(\langle\alpha|\,C^{2},0,0,\ldots)$$

Using (B12) again, one gets

$$\alpha\langle W|\,(Y-X)X=\langle W|\,(Y-X)+(\langle\alpha|\,C-\alpha\langle\alpha|\,C^2,0,...)$$

and this gives the proof for $p=1$. To prove (39) for general p, one can write

$$\alpha\langle W|\,(Y-X)\,Y^{p-1}X=\alpha\langle W|\,(Y-X)\,Y^{p-2}(YX-XY)$$
$$+\alpha\langle W|\,(Y-X)\,Y^{p-2}XY$$

Assuming that (39) is true for $p-1$, then using (B5) and (40), one finds

$$\alpha\langle W|\,(Y-X)\,Y^{p-1}X=-\alpha\langle W|\,(Y-X)\,Y^{p-2}c\psi+\langle W|\,Y^{p-2}(Y-X)\,Y$$
$$+\langle 1|\,\langle\alpha|\,c^p-\alpha\langle 1|\,\langle\alpha|\,c^{p+1}$$

and this proves (39) for p using (B5) and the fact that

$$-\alpha\langle W|\,(Y-X)\,Y^{p-2}c\psi=\langle W|\,\psi d^{p-2}c=\langle W|\,Y^{p-2}c\psi$$

which is a consequence of (B7), (B.12), (B4), (40), and (2).

APPENDIX C. EXPLICIT CALCULATIONS OF DIFFUSION CONSTANT

In this appendix we outline the ways in which we derived explicit expressions for the diffusion constant. First we recall that in order to obtain the diffusion constant one needs to compute [cf. (48), (49)]

$$\sum_{\mathscr{C}} p(\mathscr{C})\,s(\mathscr{C})=-\frac{1}{Z_N^2}\,\langle\alpha|\otimes\langle W|\,G^N\,|\beta\rangle\otimes|V\rangle \tag{C1}$$

$$\sum_{\mathscr{C},\mathscr{C}'} M_1(\mathscr{C},\mathscr{C}')\,p(\mathscr{C}')\,s(\mathscr{C})=-\frac{1}{Z_N^2}\,[(\alpha|\otimes\langle W|\,X]\,G^{N-1}\,|\beta\rangle\otimes|V\rangle \tag{C2}$$

We first introduce the notation

$$|x\rangle\;|1\rangle\;|z\rangle=|x\rangle\otimes\begin{pmatrix}|z\rangle\\0\\0\\0\\.\end{pmatrix}$$

$$|x\rangle\ |2\rangle\ |z\rangle = |x\rangle \otimes \begin{pmatrix} 0 \\ |z\rangle \\ 0 \\ 0 \\ \cdot \end{pmatrix}$$

$$|x\rangle\ |3\rangle\ |z\rangle = |x\rangle \otimes \begin{pmatrix} 0 \\ 0 \\ |z\rangle \\ 0 \\ \cdot \end{pmatrix} \cdots \tag{C3}$$

and a similar notation for the bra vectors, so that

$$|\beta\rangle \otimes |V\rangle = |\beta\rangle\ |1\rangle\ |\beta\rangle \tag{C4}$$

$$\langle\alpha| \otimes \langle W| = \sum_{i=2}^{\infty} \langle\alpha|\ \langle i|\ \langle\alpha| \tag{C5}$$

Due to the form of $G = D \otimes X + E \otimes Y$ [see Eq. (33)] one has

$$\begin{aligned} G[\,|v\rangle\ |1\rangle\ |w\rangle\,] &= D\,|v\rangle\ X[\,|1\rangle\ |w\rangle\,] + E\,|v\rangle\ Y[\,|1\rangle\ |w\rangle\,] \\ &= C\,|v\rangle\ |1\rangle\ C\,|w\rangle + D\,|v\rangle\ |2\rangle\ D\,|w\rangle \end{aligned} \tag{C6}$$

where $|v\rangle$, $|w\rangle$ are arbitrary vectors. Repeated use of (C6) implies

$$\begin{aligned} &G^m[\,|v\rangle\ |1\rangle\ |w\rangle\,] \\ &= C^m\,|v\rangle\ |1\rangle\ C^m\,|w\rangle + \sum_{n=1}^{m} G^{m-n}[DC^{n-1}\,|v\rangle\ |2\rangle\ DC^{n-1}\,|w\rangle\,] \end{aligned} \tag{C7}$$

Also, due to the form of G one has

$$[\,\langle v|\ \langle 1|\ \langle w|\,]\ G^m = \langle v|\ C^m \langle 1|\ \langle w|\ C^m \tag{C8}$$

Thus, using (C4), (C5), (C7), and (C8), one may rewrite (C1) and (C2) as

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \langle H| \sum_{n=1}^{N} G^{N-n}\,|L_n\rangle \tag{C9}$$

$$\begin{aligned} &\sum_{\mathscr{C},\mathscr{C}'} M_1(\mathscr{C},\mathscr{C}')\, p(\mathscr{C}')\, s(\mathscr{C}) \\ &= -\frac{1}{Z_N^2}\left[\langle\alpha|\ \langle 1|\ \langle\alpha|\ D + \sum_{i=2}^{\infty} \langle\alpha|\ \langle i|\ \langle\alpha|\ C\right] G^{N-1}[\,|\beta\rangle\ |1\rangle\ |\beta\rangle\,] \\ &= -\frac{\langle\alpha|\ C^{N-1}\,|\beta\rangle\langle\alpha|\ DC^{N-1}\,|\beta\rangle}{Z_N^2} - \frac{1}{Z_N^2}\langle K| \sum_{n=1}^{N-1} G^{N-1-n}\,|L_n\rangle \end{aligned} \tag{C10}$$

where $|L_n\rangle$, $\langle H|$, and $\langle K|$ are defined as

$$|L_n\rangle = DC^{n-1}\,|\beta\rangle\,|2\rangle\,DC^{n-1}\,|\beta\rangle \tag{C11}$$

$$\langle H| = \sum_{i=2}^{\infty} \langle\alpha|\,\langle i|\,\langle\alpha| \tag{C12}$$

$$\langle K| = \sum_{i=2}^{\infty} \langle\alpha|\,\langle i|\,\langle\alpha|\,C \tag{C13}$$

The action of G on $|x\rangle\,|y\rangle\,|z\rangle$ for $y \geqslant 2$ obeys the following recursion [see (33)]:

$$\begin{aligned} &G^m\,|x\rangle\,|2\rangle\,|z\rangle \\ &\quad = G^{m-1}[D\,|x\rangle\,|2\rangle\,E\,|z\rangle + D\,|x\rangle\,|3\rangle\,D\,|z\rangle + E\,|x\rangle\,|2\rangle\,D\,|z\rangle] \\ &G^m\,|x\rangle\,|y\rangle\,|z\rangle \\ &\quad = G^{m-1}[D\,|x\rangle\,|y\rangle\,E\,|z\rangle + D\,|x\rangle\,|y+1\rangle\,D\,|z\rangle \\ &\qquad + E\,|x\rangle\,|y\rangle\,D\,|z\rangle + E\,|x\rangle\,|y-1\rangle\,E\,|z\rangle] \qquad \text{for} \quad y \geqslant 3 \end{aligned} \tag{C14}$$

C1. Calculations for $\alpha = \beta = 1$

For the case $\alpha = \beta = 1$ we were able to evaluate the matrix elements of G^m required in the calculation of $\sum_{\mathscr{C}} p(\mathscr{C})\,s(\mathscr{C})$ and $\sum_{\mathscr{C},\mathscr{C}'} M_1(\mathscr{C},\mathscr{C}')\,p(\mathscr{C}')\,s(\mathscr{C})$ by choosing to work in a particular representation of the matrices, the bidiagonal choice[14]:

$$D = \sum_{x=1}^{\infty} (|x\rangle\langle x| + |x\rangle\langle x+1|); \qquad E = \sum_{x=1}^{\infty} (|x\rangle\langle x| + |x+1\rangle\langle x|) \tag{C15}$$

$$\langle\alpha| = \langle 1|; \qquad |\beta\rangle = |1\rangle \tag{C16}$$

We now list some some convenient properties of the matrices in this representations which will be useful in the calculations that follow: First we have

$$\langle 1|\,E = \langle 1|; \qquad D\,|1\rangle = |1\rangle \tag{C17}$$

$$(E-1)\,|x\rangle = |x+1\rangle; \qquad \langle x|\,(D-1) = \langle x+1| \qquad \text{for} \quad x > 0 \tag{C18}$$

which are direct consequences of the definitions (C15). A useful identity is

$$\sum_{n=1}^{i} C^{i-n} |1\rangle\langle 1| C^{n-1} = \sum_{n=1}^{i} C^{n-1} |1\rangle\langle 1| C^{i-n} = DC^i - C^iD = C^iE - EC^i \qquad \text{(C19)}$$

The first and last equalities in (C19) are trivial consequences of relabeling the sum and that $C = D + E$, respectively. That the middle equality is true for $i = 1$ is due to the fact that

$$DC - CD = DE - ED = |1\rangle\langle 1| \qquad \text{(C20)}$$

which can be checked directly from (C15), and the case of general i can easily be proved by induction. Equation (C20) may also be written as

$$E(D-1) = D - |1\rangle\langle 1| \qquad \text{and} \qquad (E-1)D = E - |1\rangle\langle 1| \qquad \text{(C21)}$$

The matrix elements of powers of C in this representation are given by [ref. 14, Eq. (35)]

$$\langle y| C^m |x\rangle = \binom{2m}{m+y-x} - \binom{2m}{m+y+x} \qquad \text{(C22)}$$

and from this formula one can check that

$$\langle 1| C^m |x+1+z\rangle = \langle x+1| C^m |z+1\rangle - \langle x| C^m |z\rangle \qquad \text{(C23)}$$

The choice of matrices (C15) also makes the particle–hole symmetry more apparent since D, E are transposes of each other. One has, for example,

$$\langle x| C^mEC^n |y\rangle = \langle y| C^nDC^m |x\rangle \qquad \text{(C24)}$$

$$\langle x| C^mE(D-E)\, C^n |y\rangle = \langle y| C^n(E-D)\, DC^m |x\rangle \qquad \text{(C25)}$$

the first of which implies

$$\sum_{n=1}^{N} \langle 1| C^{N-n}EC^{n-1} |1\rangle = \sum_{n=1}^{N} \langle 1| C^{N-n}DC^{n-1} |1\rangle = \frac{N}{2}\langle 1| C^N |1\rangle \qquad \text{(C26)}$$

and the second that

$$\begin{aligned}\langle 1| C^NE(D-E)\, C^N |1\rangle &= \tfrac{1}{2}\langle 1| C^N[E(D-E) + (E-D)D]\, C^N |1\rangle \\ &= 2\langle 1| C^{2N+1} |1\rangle - \tfrac{3}{2}\langle 1| C^N |1\rangle^2 - \tfrac{1}{2}\langle 1| C^{2N+2} |1\rangle \qquad \text{(C27)}\end{aligned}$$

where we have used $C^2 = DD + EE + ED + DE$, (C20), and $DE = C$.

Calculation for (C9) for $\alpha=\beta=1$. The matrix elements $\langle H|\, G^m\, |x\rangle\, |y\rangle\, |z\rangle$ for $y \geqslant 2$ can be explicitly computed:

$$\begin{aligned}\langle H|\, G^m\, |x\rangle\, |y\rangle\, |z\rangle \\ &= \langle 1|\, C^m\, |x\rangle \langle 1|\, C^m\, |z\rangle + \langle 1|\, C^m\, |x+y+z-1\rangle \langle 1|\, C^m\, |y-1\rangle \\ &\quad - \langle 1|\, C^m\, |y+z-1\rangle \langle 1|\, C^m\, |x+y-1\rangle \end{aligned} \tag{C28}$$

Equation (C28) may be verified by first checking that the recursion (C14) is satisfied. This can be done by noting that when any of $x=0$, $y=1$, $z=0$ holds, the r.h.s. of (C28) vanished. One then checks that when $x>0$, $y>2$, and $z>0$ each of the three terms on the r.h.s. satisfies the recursion (14) separately and that when $x>0$, $y=2$, and $z>0$ the three terms together satisfy the recursion (14). One also has to satisfy the initial conditions ($m=0$) which are dictated by the vector $\langle H|$,

$$\langle H|\, |x\rangle\, |y\rangle\, |z\rangle = \langle 1|\, |x\rangle \sum_{i=2}^{\infty} \langle i|\, |y\rangle \langle 1|\, |z\rangle = \delta_{1,x}(1-\delta_{1,y})\, \delta_{1,z} \tag{C29}$$

which agrees with setting $m=0$ in (C28). When (C28) is inserted into (C9) one obtains

$$\begin{aligned}\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \sum_{n=1}^{N} \sum_{x=1}^{\infty} \sum_{z=1}^{\infty} &[\langle 1|\, C^{N-n}\, |x\rangle \langle 1|\, C^{N-n}\, |z\rangle \\ &+ \langle 1|\, C^{N-n}\, |x+1+z\rangle \langle 1|\, C^{N-n}\, |1\rangle \\ &- \langle 1|\, C^{N-n}\, |x+1\rangle \langle 1|\, C^{N-n}\, |z+1\rangle] \\ &\times \langle x|\, DC^{n-1}\, |1\rangle \langle z|\, DC^{n-1}\, |1\rangle \end{aligned} \tag{C30}$$

In order to perform the sums over x, z one rewrites the second term in the square brackets by using (C23), then, using (C18), the particle–hole symmetry $\langle y|\, C^m E\, |x\rangle = \langle x|\, DC^m\, |y\rangle$, and the basic fact $\sum_x |x\rangle\langle x| = 1$, one obtains

$$\begin{aligned}&\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) \\ &= -\frac{1}{Z_N^2} \sum_{n=1}^{N} \{\langle 1|\, C^{N-n} DC^{n-1}\, |1\rangle^2 - \langle 1|\, C^{N-n}(E-1)\, DC^{n-1}\, |1\rangle^2 \\ &\quad + \langle 1|\, C^{N-n}\, |1\rangle \langle 1|\, C^{n-1} E[(D-1)\, C^{N-n}(E-1) - C^{N-n}]\, DC^{n-1}\, |1\rangle\} \end{aligned} \tag{C31}$$

Expression (C31) can be simplified by using (C21) and (C24),

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \sum_{n=1}^{N} \{\langle 1|\, C^{N-n} D C^{n-1}\, |1\rangle^2 - \langle 1|\, C^{N-n} E C^{n-1}\, |1\rangle^2 + \langle 1|\, C^{N-n}\, |1\rangle \times \langle 1|\, C^{n-1} [D C^{N-n} E - E C^{N-n} D]\, C^{n-1}\, |1\rangle\} \quad \text{(C32)}$$

Now, due to the particle–hole symmetry (C24) the first two sums in (C32) cancel and one is left to compute, after using $D = C - E$,

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \sum_{n=1}^{N} \langle 1|\, C^{N-n}\, |1\rangle \times [\langle 1|\, C^N E C^{n-1}\, |1\rangle - \langle 1|\, C^{n-1} E C^N\, |1\rangle] \quad \text{(C33)}$$

Using (C19), one finds

$$\begin{aligned} \sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) &= -\frac{1}{Z_N^2} [\langle 1|\, C^N E (D C^N - C^N D)\, |1\rangle - \langle 1|\, (C^N E - E C^N)\, E C^N\, |1\rangle] \\ &= -\frac{1}{Z_N^2} \langle 1|\, C^N E (D - E)\, C^N\, |1\rangle \end{aligned} \quad \text{(C34)}$$

Equation (C27) then gives

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -\frac{1}{Z_N^2} \left[2\langle 1|\, C^{2N+1}\, |1\rangle - \frac{3}{2} \langle 1|\, C^N\, |1\rangle^2 - \frac{1}{2} \langle 1|\, C^{2N+2}\, |1\rangle \right] \quad \text{(C35)}$$

Calculation of (C10) for $\alpha = \beta = 1$. The calculation of $\sum_{\mathscr{C}, \mathscr{C}'} M_1(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}')\, s(\mathscr{C})$ involves $\langle K|\, G^m\, |L_n\rangle$ [see (C10)], but since $|L_n\rangle$ given by (C11) is symmetric in its first and third components, as is the action (C14) of G, it is clear that

$$\langle K|\, G^m\, |L_n\rangle = \langle K'|\, G^m\, |L_n\rangle \quad \text{(C36)}$$

where

$$\langle K'| = \tfrac{1}{2} \left\{ \langle 1| \sum_{i=2}^{\infty} \langle i|\, \langle 1|\, C + \langle 1|\, C \sum_{i=2}^{\infty} \langle i|\, \langle 1| \right\} \quad \text{(C37)}$$

One can check that

$$\begin{aligned}
&\langle K'|\, G^m\, |x\rangle\, |y\rangle\, |z\rangle \\
&\quad =\tfrac{1}{2}\{\langle 1|\, C^m\, |x\rangle\langle 1|\, C^{m+1}\, |z\rangle+\langle 1|\, C^m\, |z\rangle\langle 1|\, C^{m+1}\, |x\rangle \\
&\qquad +\langle 1|\, C^m\, |x+y+z-1\rangle\langle 1|\, C^{m+1}\, |y-1\rangle \\
&\qquad +\langle 1|\, C^m\, |y-1\rangle\langle 1|\, C^{m+1}\, |x+y+z-1\rangle \\
&\qquad -\langle 1|\, C^m\, |y+z-1\rangle\langle 1|\, C^{m+1}\, |x+y-1\rangle \\
&\qquad -\langle 1|\, C^m\, |x+y-1\rangle\langle 1|\, C^{m+1}\, |y+z-1\rangle\}
\end{aligned} \tag{C38}$$

satisfies the recursion (C14) and initial conditions $(m=0)$

$$\begin{aligned}
\langle K'|\, |x\rangle\, |y\rangle\, |z\rangle &=\tfrac{1}{2}\{\langle 1|\, |x\rangle\langle 1|\, C\, |z\rangle+\langle 1|\, |z\rangle\langle 1|\, C\, |x\rangle\} && \text{if}\quad y\geqslant 2 \\
&=0 && \text{if}\quad y=1
\end{aligned}$$

Performing the sums over x and z as was done to obtain (C31), one finds

$$\begin{aligned}
&\sum_{n=1}^{N-1}\langle K'|\, G^{N-n-1}\, |L_n\rangle \\
&\quad =\tfrac{1}{2}\sum_{n=1}^{N-1}\{2\langle 1|\, C^{N-1-n}DC^{n-1}\, |1\rangle\langle 1|\, C^{N-n}DC^{n-1}\, |1\rangle \\
&\qquad -2\langle 1|\, C^{N-1-n}(E-1)\, DC^{n-1}\, |1\rangle\langle 1|\, C^{N-n}(E-1)\, DC^{n-1}\, |1\rangle \\
&\qquad +\langle 1|\, C^{N-n}\, |1\rangle \\
&\qquad \times\langle 1|\, C^{n-1}E[(D-1)\, C^{N-1-n}(E-1)-C^{N-1-n}]\, DC^{n-1}\, |1\rangle \\
&\qquad +\langle 1|\, C^{N-1-n}\, |1\rangle \\
&\qquad \times\langle 1|\, C^{n-1}E[(D-1)\, C^{N-n}(E-1)-C^{N-n}]\, DC^{n-1}\, |1\rangle\}
\end{aligned} \tag{C39}$$

Expression (C39) can be simplified using (C21) and (C24),

$$\begin{aligned}
&\sum_{n=1}^{N-1}\langle K'|\, G^{N-n-1}\, |L_n\rangle \\
&\quad =\sum_{n=1}^{N-1}\{\langle 1|\, C^{N-1-n}DC^{n-1}\, |1\rangle\langle 1|\, C^{N-n}DC^{n-1}\, |1\rangle \\
&\qquad -\langle 1|\, C^{N-1-n}EC^{n-1}\, |1\rangle\langle 1|\, C^{N-n}EC^{n-1}\, |1\rangle \\
&\qquad +\tfrac{1}{2}\langle 1|\, C^{N-n}\, |1\rangle\langle 1|\, C^{n-1}[DC^{N-1-n}E-EC^{N-1-n}D]\, C^{n-1}\, |1\rangle \\
&\qquad +\tfrac{1}{2}\langle 1|\, C^{N-1-n}\, |1\rangle\langle 1|\, C^{n-1}[DC^{N-n}E-EC^{N-n}D]\, C^{n-1}\, |1\rangle\}
\end{aligned} \tag{C40}$$

The first two sums in (C40) may be computed using $D=C-E$ and (C26),

$$\sum_{n=1}^{N-1} \{\langle 1|\, C^{N-1-n}DC^{n-1}\,|1\rangle\langle 1|\, C^{N-n}DC^{n-1}\,|1\rangle$$
$$-\langle 1|\, C^{N-1-n}EC^{n-1}\,|1\rangle\langle 1|\, C^{N-n}EC^{n-1}\,|1\rangle\}$$
$$=\sum_{n=1}^{N-1} \{\langle 1|\, C^{N-1}\,|1\rangle\langle 1|\, C^{N}\,|1\rangle-\langle 1|\, C^{N-1}\,|1\rangle\langle 1|\, C^{N-n}EC^{n-1}\,|1\rangle$$
$$-\langle 1|\, C^{N}\,|1\rangle\langle 1|\, C^{N-1-n}EC^{n-1}\,|1\rangle\}$$
$$=\langle 1|\, C^{N-1}\,|1\rangle^2-\tfrac{1}{2}\langle 1|\, C^{N}\,|1\rangle\langle 1|\, C^{N-1}\,|1\rangle \tag{C41}$$

The last two sums is (C40) may be evaluated by using (19), after using $D=C-E$:

$$\tfrac{1}{2}\sum_{n=1}^{N} \langle 1|\, C^{N-n}\,|1\rangle[\langle 1|\, C^{N-1}EC^{n-1}\,|1\rangle-\langle 1|\, C^{n-1}EC^{N-1}\,|1\rangle]$$
$$+\tfrac{1}{2}\sum_{n=1}^{N-1} \langle 1|\, C^{N-1-n}\,|1\rangle[\langle 1|\, C^{N}EC^{n-1}\,|1\rangle-\langle 1|\, C^{n-1}EC^{N}\,|1\rangle]$$
$$=\tfrac{1}{2}\langle 1|\, C^{N-1}E[DC^N-C^ND]\,|1\rangle-\tfrac{1}{2}\langle 1|\,[C^NE-EC^N]\,EC^{N-1}\,|1\rangle$$
$$+\tfrac{1}{2}\langle(1|\, C^NE[DC^{N-1}-C^{N-1}D]\,|1\rangle$$
$$-\tfrac{1}{2}\langle 1|\,[C^{N-1}E-EC^{N-1}]\,EC^N\,|1\rangle$$
$$=\tfrac{1}{2}\langle 1|\, C^{N-1}E(D-E)\,C^N\,|1\rangle-\tfrac{1}{2}\langle 1|\, C^NE(E-D)\,C^{N-1}\,|1\rangle$$
$$=\tfrac{1}{2}\langle 1|\, C^{N-1}E(D-E)\,C^N\,|1\rangle-\tfrac{1}{2}\langle 1|\, C^{N-1}(D-E)\,DC^N\,|1\rangle$$
$$=2\langle 1|\, C^{2N}\,|1\rangle-\tfrac{3}{2}\langle 1|\, C^{N-1}\,|1\rangle\langle 1|\, C^N\,|1\rangle-\tfrac{1}{2}\langle 1|\, C^{2N+1}\,|1\rangle \tag{C42}$$

Putting (C10) and (C40)–(C42) together, one obtains

$$\sum_{\mathscr{C},\mathscr{C}'} M_1(\mathscr{C},\mathscr{C}')\,p(\mathscr{C}')\,s(\mathscr{C})$$
$$=-\frac{1}{Z_N^2}\left[2\langle 1|\, C^{2N}\,|1\rangle-\frac{1}{2}\langle 1|\, C^{2N+1}\,|1\rangle-\langle 1|\, C^N\,|1\rangle\langle 1|\, C^{N-1}\,|1\rangle\right] \tag{C43}$$

Calculation of Δ for $\alpha=\beta=1$. The diffusion constant is given by [cf. (24)]

$$\Delta=J+2\sum_{\mathscr{C},\mathscr{C}'} M_1(\mathscr{C},\mathscr{C}')\,p(\mathscr{C}')\,s(\mathscr{C})-2J\sum_{\mathscr{C}} p(\mathscr{C})\,s(\mathscr{C}) \tag{C44}$$

Using (C35) and (C43) and recalling that $J = Z_{N-1}/Z_N$ and $Z_N = \langle 1|\, C^N \,|1\rangle$, one obtains

$$\Delta = \frac{2}{\langle 1|\, C^N \,|1\rangle^3} \left\{ \langle 1|\, C^{N-1} \,|1\rangle \left[2\langle 1|\, C^{2N+1} \,|1\rangle - \frac{1}{2} \langle 1|\, C^{2N+2} \,|1\rangle \right] \right.$$
$$\left. - \langle 1|\, C^N \,|1\rangle \left[2\langle 1|\, C^{2N} \,|1\rangle - \frac{1}{2} \langle 1|\, C^{2N+1} \,|1\rangle \right] \right\} \tag{C45}$$

Now (C22) gives

$$\langle 1|\, C^N \,|1\rangle = \frac{(2N+2)!}{(N+2)!\,(N+1)!} \tag{C46}$$

and using this, one can check that (C45) simplifies to

$$\Delta = \frac{3(4N+1)!\,[N!\,(N+2)!]^2}{2[(2N+1)!]^3\,(2N+3)!} \tag{C47}$$

This result is the same as that conjectured in ref. 25, up to a factor $1/(N+1)$, which had been forgotten in Eq. 49 of ref. 25.

C.2. The Case $\alpha + \beta = 1$

In this case it is known that the matrices D and E can be chosen as scalars[14]

$$D = \frac{1}{\beta}; \qquad E = \frac{1}{\alpha}$$

Therefore we have

$$C = \frac{1}{\alpha} + \frac{1}{\beta} = \frac{1}{\alpha\beta} \qquad \text{and} \qquad J = \alpha\beta$$

The matrices X and Y are then simply infinite matrices with scalar elements:

$$X = \begin{pmatrix} 1/\alpha\beta & 0 & 0 & 0 & \cdot & \cdot \\ 1/\beta & 1/\alpha & 0 & & & \\ 0 & 1/\beta & 1/\alpha & & & \\ 0 & 0 & 1/\beta & 1/\alpha & & \\ \cdot & & & & \cdot & \\ \cdot & & & & & \cdot \end{pmatrix}, \quad Y = \begin{pmatrix} 1/\alpha\beta & 0 & 0 & 0 & \cdot & \cdot \\ 0 & 1/\beta & 1/\alpha & 0 & & \\ 0 & 0 & 1/\beta & 1/\alpha & & \\ 0 & 0 & 0 & 1/\beta & & \\ \cdot & & & & \cdot & \\ \cdot & & & & & \cdot \end{pmatrix}$$

$$\langle W| = (0,\ 1,\ 1\ \cdot\ \cdot) = \sum_{i=2}^{\infty} \langle i|, \qquad |V\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \cdot \\ \cdot \end{pmatrix} = |1\rangle$$

and $G = D \otimes X + E \otimes Y$ is simply $(1/\beta) X + (1/\alpha) Y$.

It will be convenient to introduce the matrix $T = (\alpha\beta)^2 G$,

$$T = (\alpha\beta)^2 \left(\frac{1}{\beta} X + \frac{1}{\alpha} Y\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdot \\ \alpha^2 & 2\alpha\beta & \beta^2 & 0 & 0 & \\ 0 & \alpha^2 & 2\alpha\beta & \beta^2 & 0 & \\ 0 & 0 & \alpha^2 & 2\alpha\beta & \beta^2 & \\ \cdot & & & & \cdot & \cdot \\ \cdot & & & & & \cdot \end{pmatrix} \tag{C48}$$

The two sums to be computed in the expression of Δ [see (24)] then take the following forms:

$$\sum_{\mathscr{C}} p(\mathscr{C})\, s(\mathscr{C}) = -(\alpha\beta)^{2N} \langle W| \left(\frac{1}{\beta} X + \frac{1}{\alpha} Y\right)^N |V\rangle = -\langle W| T^N |V\rangle \tag{C49}$$

$$\begin{aligned} \sum_{\mathscr{C}, \mathscr{C}'} M_1(\mathscr{C}, \mathscr{C}')\, p(\mathscr{C}')\, s(\mathscr{C}) &= -(\alpha\beta)^2 \langle W|\, X T^{N-1} |V\rangle \\ &= -(\alpha\beta)^2 \left\{ \frac{1}{\beta} \langle 1|\, T^{N-1} |1\rangle - \frac{1}{\alpha\beta} \langle W|\, T^{N-1} |V\rangle \right\} \\ &= -\alpha^2\beta - (\alpha\beta) \langle W|\, T^{N-1} |V\rangle \end{aligned} \tag{C50}$$

To obtain the last two equalities we used the fact that $\langle W| X = (1/\beta)\langle 1| + (1/\alpha\beta)\langle W|$ and that $\langle 1|$ is an eigenvector of T. One finally derives the expression for Δ,

$$\Delta = \alpha\beta + 2\alpha\beta\{\langle W|\, T^N |V\rangle - \langle W|\, T^{N-1} |V\rangle - \alpha\} \tag{C51}$$

The matrix element $\langle W|\, T^N |V\rangle$ can be calculated with the help of generating functions:

$$F_k(\lambda) = \sum_{n=0}^{\infty} \langle k|\, T^n |V\rangle\, \lambda^n$$

These functions satisfy the following recursion:

$$F_1(\lambda) = \frac{1}{1-\lambda}$$

$$F_k(\lambda) = \lambda\{\alpha^2 F_{k-1}(\lambda) + 2\alpha\beta F_k(\lambda) + \beta^2 F_{k+1}(\lambda)\} \qquad \text{for} \quad k \geqslant 2$$

The solution of this recursion is readily found:

$$F_k(\lambda) = \frac{r^{k-1}}{1-\lambda} \qquad \text{with} \quad r = \frac{1 - 2\alpha\beta\lambda - (1 - 4\alpha\beta\lambda)^{1/2}}{2\beta^2\lambda}$$

Thus the term $\langle W|\, T^N \,|V\rangle$ is the coefficient of λ^N in

$$\sum_{k=2}^{\infty} F_k(\lambda) = -\frac{1}{1-\lambda} + \frac{1}{(1-\lambda)(1-r)}$$

which, using $\alpha + \beta = 1$,

$$\frac{1 - (1-4x)^{1/2}}{2x} = \sum_{n=0}^{\infty} \frac{(2n)!}{n!\,(n+1)!}\, x^n$$

is found to be

$$\langle W|\, T^N \,|V\rangle = N\alpha - \alpha\beta \sum_{k=0}^{N-1} (N-k) \frac{(2k)!}{k!\,(k+1)!} (\alpha\beta)^k$$

After substituting this coefficient in (C51), one obtains the following expression for Δ:

$$\Delta = \alpha\beta - 2(\alpha\beta)^2 \sum_{k=0}^{N-1} (\alpha\beta)^k \frac{(2k)!}{k!\,(k+1)!}$$

Or, equivalently,

$$\Delta = J\left(1 - 2J \sum_{k=0}^{N-1} \frac{(2k)!}{k!\,(k+1)!} J^k\right) \tag{C52}$$

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