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Matrix-Product States for a One-Dimensional Lattice Gas with Parallel Dynamics

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Abstract

The hopping motion of classical particles on a chain coupled to reservoirs at both ends is studied for parallel dynamics with arbitrary probabilities. The stationary state is obtained in the form of an alternating matrix product. The properties of one- and two-dimensional representations are studied in detail and a general relation of the matrix algebra to that of the sequential limit is found. In this way the general phase diagram of the model is obtained. The mechanism of the sequential limit, the formulation as a vertex model and other aspects are discussed.

Keywords: Kinetic models, parallel dynamics, boundary effects, spin chains, vertex models, matrix-product states

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1. Introduction

The study of classical kinetic models in one dimension has revealed interesting physical properties (e.g. non-equilibrium phase transitions) and mathematical structures. Moreover, one finds close connections with quantum-mechanical spin problems. A prominent example is the diffusion of particles with hard-core repulsion on the sites of a chain which is coupled to reservoirs at both ends [1 – 4]. This model shows at least three phases which differ in their density profiles and the current through the system. Boundary effects, i.e. the rates at which particles enter and leave the system, play an essential rôle. Mathematically, the model can be described as a spin one-half problem and, if the dynamics consists of single particle processes, the time evolution operator of the master equation has the form of the Hamiltonian of the Heisenberg model with boundary fields at both ends. The stationary state can be written in the form of a matrix product, where the weight of a configuration is given by an expression of the form $\langle W|ABBAB\ldots|V\rangle$ with operators A, B and vectors $\langle W|$, $|V\rangle$ in an auxiliary space. Such states, which generalize simple product states so as to give non-trivial correlations, were first found in a problem of lattice animals [5] and for certain quantum spin chains [6, 7]. They have also been encountered in diffusion-coagulation models [8]. The detailed mechanism is somewhat different in each of the three cases.

In the following we will study this model with a more general type of dynamics. The time is taken discrete and in each time step, hopping processes between half of all pairs of nearest-neighbour sites can take place. This is not yet full parallel dynamics as desired e.g. in traffic-flow problems, but we will still term it 'parallel'. This model has been considered before in the case of deterministic uni-directional motion on the chain [9]. Here we will treat the general case where the particles hop with probabilities p and q to the right and left, respectively. This contains the deterministic as well as the sequential dynamics of the master equation as special cases. The latter is obtained if all probabilities tend towards zero. This limiting case corresponds to the Hamiltonian limit in two-dimensional statistical physics. In fact, there is a close relation to that area, since the parallel dynamics can be formulated as an asymmetric six-vertex model with additional boundary terms.

It turns out that this general model has properties which are quite similar to those of the sequential limit. One physical distinction is a stationary density which alternates from site to site and which results from the boundary terms combined with the structure of our parallel dynamics. The matrix-product groundstate, which also exists here, has a corresponding sublattice structure. The mechanism for the stationary state is the same as already encountered in the deterministic limit $p = 1$, $q = 0$ [9]. In each time step (corresponding to the action of one row of vertices in the vertex model), the sublattices exchange their rôle, so that after two steps the state is reproduced. It should be mentioned that simple (scalar) product states in two-dimensional models were studied already some time ago. For example, a homogeneous state of that type was found for special cases of eight-vertex models with fields [10]. Alternating states were considered in [11, 12] for the case of IRF models which are the dual formulation of vertex models. In the context of spin systems, such states are called 'disorder solutions' and usually result from competing interactions (see [13] and references therein).

To obtain the stationary state, one may try to find a finite-dimensional representation of the four operators defining the algebra and the corresponding vectors satisfying the boundary

relations. Here we present a scalar product state (i.e. a one-dimensional representation) and a representation in terms of two-dimensional matrices. These representations exist for special submanifolds in the parameter space. The general situation, however, is more easily handled if one notes that there exist representations where the quantities on one sublattice may be eliminated such that one can lift any representation of the algebra in the sequential limit with suitably 'renormalized' parameters to a representation of the algebra for parallel dynamics. This feature has also been discovered independently in the context of a dynamics where the updating is done step-by-step from one end of the chain to the other [14] [1]). Using this connection, we can take over results and methods for the sequential case, e.g. to calculate the current or the density profile in the general case. In this way, one obtains a rather complete picture.

The paper is organized as follows. In Section 2 we introduce the model, discuss the vertex formulation, the Hamiltonian limit, and set up relations for the matrix-product state. In Section 3 we find one- and two-dimensional matrix representations for the algebra arising from the matrix-product ansatz which we use in Section 4 to compute various physical quantities. The mapping to the sequential case is described in Section 5 and used in Section 6 to compute the current for general values of the parameters. Section 7 contains a discussion of the results and remarks on some other aspects as the relation to the model in [14] and the integrability of the model. Several appendices contain some supplementary material.

2. Model and matrix-product ansatz

The diffusion of particles with hard-core repulsion is a stochastic process on a lattice which we here choose to be one-dimensional with N sites where N is even. Each site can have two states: It can either be empty or it can be occupied by one particle. Particles can hop along the bonds of the lattice onto empty sites, to the right with probability p and to the left with probability q. At the left and right boundaries particles can be added or extracted. Particles are added to an empty leftmost site with probability α and removed from it with probability γ. At the right boundary they are extracted with probability β and added with probability δ. All theses processes can take place simultaneously, but updates are performed in two steps in order to permit at most one hopping process at each site in any time step. Particles are removed and added at the boundaries during the first time step. During this time step they can also hop along the bonds connecting the even sites with the odd ones to their right. During the second time step they can hop only along the other bonds. Because of the restriction that a site may be occupied by at most one particle, this is a non-trivial many-body problem.

For these update rules the time transfer matrix T which describes the time evolution of the probability distribution has the structure $T = T_2 T_1$ where T_1 accounts for all processes that can take place during the first time step, and T_2 for those of the second one. They

[1]) In this paper we will use a different terminology than in [14]. We reserve the term 'sequential' for a situation where in each time step only one local process can take place, but at a random position.

are given by

$$T_1 = \mathcal{L} \otimes \underbrace{\mathcal{T} \otimes \cdots \otimes \mathcal{T}}_{N-1 \text{ times}} \otimes \mathcal{R}\,,$$
$$T_2 = \underbrace{\mathcal{T} \otimes \mathcal{T} \otimes \cdots \otimes \mathcal{T}}_{N \text{ times}}\,, \tag{2.1}$$

where the matrices $\mathcal{T}$, $\mathcal{L}$ and $\mathcal{R}$ describe hopping and particle input and output, respectively. In a suitable basis they are given by

$$\mathcal{T} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1-q & p & 0 \\ 0 & q & 1-p & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \qquad \mathcal{L} = \begin{pmatrix} 1-\alpha & \gamma \\ \alpha & 1-\gamma \end{pmatrix}, \qquad \mathcal{R} = \begin{pmatrix} 1-\delta & \beta \\ \delta & 1-\beta \end{pmatrix}. \tag{2.2}$$

This stochastic model can be regarded as a vertex model with the time evolution operator T corresponding to the diagonal-to-diagonal transfer matrix [15, 16]. This is shown in Fig. 1 where the particles sit on the bonds of the lattice and time evolves upwards. The initial state before application of T is given by the configuration of the bonds at the lower edge of the shaded region, and the final state is given by that at its upper border.

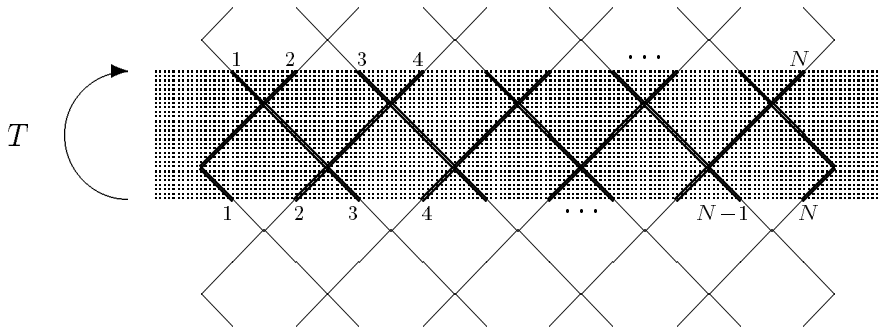


Fig. 1: Representation of the hopping processes as a vertex model. Only a part of the lattice is shown in the vertical direction. The shaded region contains all vertices that contribute to the diagonal-to-diagonal transfer matrix T.

The local update operators (2.2) can then be reinterpreted in terms of the Boltzmann weights of all possible vertex configurations as shown in Fig. 2 where the presence (absence) of a particle on a bond is indicated by an arrow pointing upwards (downwards). This vertex model is somewhat more complicated than the one treated in [17]. Usually, one considers the symmetric six-vertex model which is invariant under inversion of the arrows (i.e. particle-hole symmetry). For $p \neq q$ the bulk vertices in the first line of Fig. 2 do not have this symmetry. More importantly, the boundary vertices in the second line do not conserve the particle number, because they correspond to particle injection and extraction.

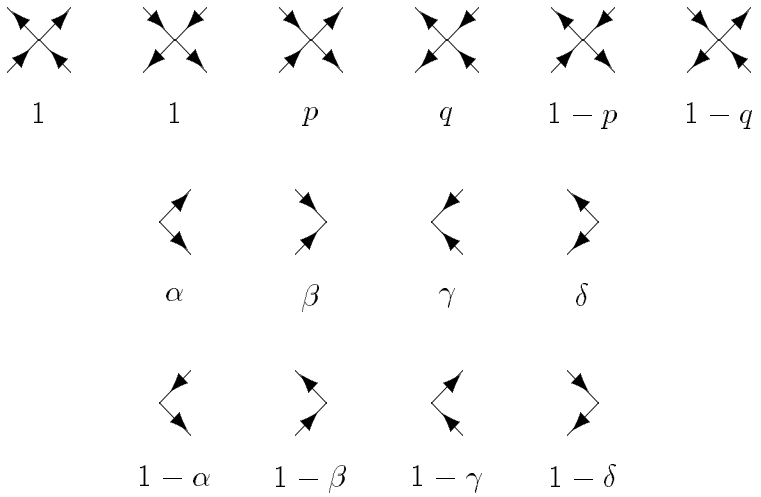


Fig. 2: The Boltzmann weights for the vertex model describing hopping with parallel dynamics.

In this paper we shall be interested in the stationary state, i.e. a state that is invariant under the time evolution operator T. In the language of the vertex model this corresponds to the 'groundstate' of the diagonal-to-diagonal transfer matrix.

Because of the sublattice structure of the transfer matrix (2.1) we make an alternating matrix-product ansatz for the stationary state

$$\langle W| \begin{pmatrix} A \\ B \end{pmatrix} \otimes \begin{pmatrix} \widehat{A} \\ \widehat{B} \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} A \\ B \end{pmatrix} \otimes \begin{pmatrix} \widehat{A} \\ \widehat{B} \end{pmatrix} |V\rangle \,, \tag{2.3}$$

where A, B, $\widehat{A}$ and $\widehat{B}$ are operators in an auxiliary space. The operators A and $\widehat{A}$ describe empty places while B and $\widehat{B}$ encode the presence of a particle. $|V\rangle$ and $|W\rangle$ are vectors in this auxiliary space which have to be chosen suitably and have to satisfy the condition $\langle W|V\rangle \neq 0$ in order for (2.3) to be non-zero.

The mechanism of [9] (and similarly [12]) assumes that T_1 as well as T_2 exchange the operators A, B and $\widehat{A}$, $\widehat{B}$ with each other. At the boundaries this gives rise to the conditions

$$\langle W|\mathcal{L} \begin{pmatrix} A \\ B \end{pmatrix} = \langle W| \begin{pmatrix} \widehat{A} \\ \widehat{B} \end{pmatrix} , \qquad \mathcal{R} \begin{pmatrix} \widehat{A} \\ \widehat{B} \end{pmatrix} |V\rangle = \begin{pmatrix} A \\ B \end{pmatrix} |V\rangle \tag{2.4}$$

and for the interior one has

$$\mathcal{T} \left\{ \begin{pmatrix} \widehat{A} \\ \widehat{B} \end{pmatrix} \otimes \begin{pmatrix} A \\ B \end{pmatrix} \right\} = \begin{pmatrix} A \\ B \end{pmatrix} \otimes \begin{pmatrix} \widehat{A} \\ \widehat{B} \end{pmatrix} . \tag{2.5}$$

After inserting the matrices (2.2), this ansatz leads to

$$\begin{aligned} \widehat{A}A = A\widehat{A} \,, \qquad & (1-q)\widehat{A}B + p\widehat{B}A = A\widehat{B} \,, \\ \widehat{B}B = B\widehat{B} \,, \qquad & q\widehat{A}B + (1-p)\widehat{B}A = B\widehat{A} \,, \end{aligned} \tag{2.6a}$$

$$\begin{aligned} \{(1-\delta)\widehat{A} + \beta\widehat{B}\}|V\rangle = A|V\rangle \,, \qquad & \{\delta\widehat{A} + (1-\beta)\widehat{B}\}|V\rangle = B|V\rangle \,, \\ \langle W|\{(1-\alpha)A + \gamma B\} = \langle W|\widehat{A} \,, \qquad & \langle W|\{\alpha A + (1-\gamma)B\} = \langle W|\widehat{B} \,. \end{aligned} \tag{2.6b}$$

It has been argued in [9] that the relations (2.6) define a consistent associative algebra with Fock representation. However, so far the problem of finding the groundstate of T has just been reformulated and not yet been solved. In order to make further progress, one needs a representation of the algebra defined by the A, B, $\widehat{A}$ and $\widehat{B}$ with suitable additional properties. This will be the subject of Sections 3 and 5.

The corresponding matrix-product state of the sequential limit is well-known (see e.g. [3, 18, 19]). The sequential limit is the limit of small probabilities, or equivalently the Hamiltonian limit in the language of vertex models. In order to be more precise set

$$x := \rho\,\widehat{x} \tag{2.7}$$

for $x = p, q, \alpha, \beta, \gamma, \delta$ such that one can make an expansion in powers of ρ. An immediate consequence of the definitions is that

$$\mathcal{T} = \mathbb{1} - \rho\, h\,, \qquad \mathcal{L} = \mathbb{1} - \rho\, h_L\,, \qquad \mathcal{R} = \mathbb{1} - \rho\, h_R\,, \tag{2.8}$$

with matrices h, h_L and h_R that are independent of ρ and describe the local processes with rates $\widehat{p}$, $\widehat{q}$, $\widehat{\alpha}$, $\widehat{\beta}$, $\widehat{\gamma}$ and $\widehat{\delta}$. The transfer matrix T now takes the form

$$T = \mathbb{1} - \rho\, H + \mathcal{O}(\rho^2)\,, \tag{2.9}$$

where the Hamiltonian H contains only nearest-neighbour interactions. After a similarity transformation, this Hamiltonian becomes the $U_q(su(2))$-invariant Hamiltonian of the ferromagnetic XXZ-Heisenberg model [20] with additional boundary terms h_L and h_R (see e.g. [19]). Since this Hamiltonian does not have any sublattice structure one can make a homogenous matrix-product ansatz. We set $A = \widehat{A} = E$ and $B = \widehat{B} = D$ such that the operators with and without hat in (2.3) become equal. Then one imposes the following relations [3, 18, 19] (see also [8]) at the boundaries

$$\langle W| h_L \begin{pmatrix} E \\ D \end{pmatrix} = \langle W| \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \qquad h_R \begin{pmatrix} E \\ D \end{pmatrix} |V\rangle = -\begin{pmatrix} -1 \\ 1 \end{pmatrix} |V\rangle\,, \tag{2.10}$$

and the following algebra for the bulk

$$h\left\{\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}\right\} = \left\{\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} -1 \\ 1 \end{pmatrix} - \begin{pmatrix} -1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}\right\}. \tag{2.11}$$

With this ansatz the right term in (2.11) at site x cancels the left term at site $x+1$ if the complete Hamiltonian is applied. Finally, one is left with two boundary terms which are cancelled by (2.10).

After inserting the explicit matrices h, h_L and h_R one finds that (2.10) and (2.11) are equivalent to

$$\begin{aligned} \widehat{p}DE - \widehat{q}ED &= D + E\,, \\ \left(\widehat{\beta}D - \widehat{\delta}E\right)|V\rangle &= |V\rangle\,, \\ \langle W|\left(\widehat{\alpha}E - \widehat{\gamma}D\right) &= \langle W|\,. \end{aligned} \tag{2.12}$$

This algebra can be used to compute expectation values in the stationary state efficiently by means of recurrence relations (see [3, 18, 19]). The operator $C := E + D$ acts like a transfer matrix in the spatial direction. Obviously, $\langle W|C^N|V\rangle$ is the sum of all coefficients of the groundstate. In order to obtain a probability distribution one has to divide by this factor. Then e.g. the density profile $\langle\tau_x\rangle$ is given by the expectation values $\langle\tau_x\rangle = \langle W|C^{x-1}DC^{N-x}|V\rangle/\langle W|C^N|V\rangle$.

One of the main motivations for the work to be reported below was to find out how the mechanism (2.4), (2.5) is related to the known mechanism (2.10), (2.11) in the sequential limit. In the next Section we will first see what the relation is in two special cases.

3. One- and two-dimensional representations

First we consider a *scalar* product state. For this representation of the algebra (2.6) the operators A, B, $\widehat{A}$ and $\widehat{B}$ are mapped to real numbers a, b, $\widehat{a}$ and $\widehat{b}$ and the boundary vectors can be discarded. (We do not write the representation map explicitly and below we will also use the same notation for the algebra and its representation). After fixing the normalization suitably, the condition (2.6b) is equivalent to

$$\begin{aligned} a &= \delta\gamma - \gamma - \beta + \beta\gamma\,, \qquad & b &= \delta\alpha - \alpha - \delta + \beta\alpha\,, \\ \widehat{a} &= \beta\gamma - \gamma - \beta + \beta\alpha\,, \qquad & \widehat{b} &= \delta\gamma - \alpha - \delta + \delta\alpha\,. \end{aligned} \tag{3.1}$$

The bulk relations (2.6a) are satisfied if $(1-q)\widehat{a}b - (1-p)\widehat{b}a = 0$. Inserting the result (3.1) one finds that the probabilities p, q, α, β, γ and δ have to obey the relation

$$\begin{aligned} &(1-q)(\beta\gamma - \gamma - \beta + \beta\alpha)(\delta\alpha - \alpha - \delta + \beta\alpha) \\ &= (1-p)(\delta\gamma - \alpha - \delta + \delta\alpha)(\delta\gamma - \gamma - \beta + \beta\gamma)\,. \end{aligned} \tag{3.2}$$

Note that this condition is symmetric under the exchange of p with q, α with δ and β with γ. This symmetry is to be expected because parity (reflection at the centre of the chain) effects precisely this exchange of the probabilities. A further expansion of (3.2) is not very enlightning, but a few special cases may be worth while mentioning. For $\gamma = \delta = 0$ but $\alpha \neq 0 \neq \beta$ the relation (3.2) specializes to

$$(1-q)(\alpha + \beta - \alpha\beta) = p - q\,. \tag{3.3}$$

This condition agrees with the one that has been found in [14] for the existence of a one-dimensional representation with $\gamma = \delta = 0$. Another interesting case is the sequential limit. This is obtained by inserting (2.7) into (3.2) and keeping only the leading non-trivial order in ρ. As expected, one obtains a condition that is equivalent to the known result for sequential dynamics, namely eq. (78) in [19].

We would like to conclude the discussion of the one-dimensional representation with a remark on more general mechanisms than (2.4), (2.5). Firstly, one can get rid of the alternating structure in space by introducing a four-state model that uses block-spin variables for the states on any odd site and the even site to its right. Then one can make a homogenous product state ansatz. If one further requires the coefficients of this state to be independent of N for all even $N \geq 2$, one finds that the relation (3.2) must be satisfied.

Even more strongly, one finds that the block-spin product state can be factorized in the product state that we have already found above. In this sense, the mechanism (2.4), (2.5) gives rise to the most general scalar product state.

Now we turn to the more interesting case of a *two-dimensional* matrix-product state. As we have already indicated at the end of the previous Section, the matrices

$$C := A + B\,, \qquad \widehat{C} := \widehat{A} + \widehat{B}\,, \tag{3.4}$$

will play the rôle of transfer matrices in space. Therefore, it is desirable to find representations where C and $\widehat{C}$ have a particularly simple form. First one observes by summing over the columns in (2.5) that $[C, \widehat{C}] = 0$. Since C and $\widehat{C}$ commute they can be simultaneously brought into diagonal –or more generally– Jordan normal form. If C and $\widehat{C}$ are both invertible, an even more stronger statement holds [9], namely that one can find an equivalent representation where $C = \widehat{C}$. On the other hand, one can check that any non-trivial two-dimensional representation where $C \neq c\,\widehat{C}$ with some constant c leads to the condition (3.2) and is therefore not interesting. For this reason we will from now on only consider representations where

$$C = \widehat{C}\,. \tag{3.5}$$

This choice also ensures that half of the boundary equations (2.4) are satisfied automatically.

First we consider representations where $C = \widehat{C}$ can be diagonalized. We fix the normalization of the representation by requiring that $C_{1,1} = 1$. So, apart from the matrix elements e.g. of A and $\widehat{A}$ (and the vectors $|V\rangle$, $|W\rangle$), only $C_{2,2}$ is still free. With this choice we first solve the bulk equations (2.6a). One solution is given by

$$\begin{aligned}
C = \widehat{C} &= \begin{pmatrix} 1 & 0 \\ 0 & -\frac{(\mathcal{A}(p-q)(p+q-1)+p(1-p))(\mathcal{A}(p-q)-p)}{(\mathcal{A}(p-q)-p+1)pq} \end{pmatrix}, \\
A &= \begin{pmatrix} -\frac{\mathcal{A}(q-1)}{\mathcal{A}(p-q)-p+1} & 1 \\ 0 & \frac{(q-1)(\mathcal{A}(p-q)-p)\mathcal{A}}{(\mathcal{A}(p-q)-p+1)p} \end{pmatrix}, \\
\widehat{A} &= \begin{pmatrix} \mathcal{A} & 1 \\ 0 & \frac{\mathcal{A}(\mathcal{A}(p-q)(p+q-1)+p(1-p))}{(\mathcal{A}(p-q)-p+1)p} \end{pmatrix},
\end{aligned} \tag{3.6}$$

where the constant $\mathcal{A}$ remains free. In obtaining (3.6) we have used the freedom to rescale the two basis vectors in the representation space independently to set $\widehat{A}_{1,2} = 1$.

Now we have to solve the boundary equations (2.6b). Non-trivial solutions for the vectors $|V\rangle$ and $|W\rangle$ exist iff

$$\det\left((1-\alpha)A + \gamma B - \widehat{A}\right) = 0 = \det\left((1-\delta)\widehat{A} + \beta\widehat{B} - A\right). \tag{3.7}$$

The solution of (3.7) can be reduced to a discussion of the diagonal elements since all matrices in (3.6) are upper triangular. The relevant solution is given by the vanishing of

the (1,1)-element in the left matrix and the (2,2)-element of the right one. From this one first finds that the constant $\mathcal{A}$ is given by

$$\begin{aligned}\mathcal{A} =&\big((1-p)\,(pq\gamma+q\delta\,\gamma\,(1-p-q)+p\beta\,(p+\gamma\,(1-p-q))))\\ &\big(q\delta\,(1-q)\,(q\,(1-\alpha)+\alpha+\gamma)+p\beta\,(1-p)\,(p\,(1-\gamma)+\alpha+\gamma)+\\ &pq\,((1-2\,\delta-\beta)\,\gamma+(1-2\,\beta-\delta)\,\alpha)+pq\,((q\alpha+p\gamma)\,(\beta+\delta-1)+q\gamma\,\delta+p\alpha\,\beta)\big)^{-1}\,,\end{aligned} \tag{3.8}$$

and with this result the following relation between the parameters of the model:

$$\begin{aligned}&(1-p)\,(1-q)\,\left(p^3\alpha^2\beta^2-q^3\gamma^2\delta^2\right)\\ &+(1-p)\,pq^2\gamma\delta\,\Big(\alpha\beta\,(1-q)^2+(1-q)\,(q\,(\alpha+\beta)-(\delta\alpha+\beta\gamma))-q\,((1-\gamma)\,\delta+\gamma-q)\Big)\\ &-(1-q)\,p^2q\alpha\beta\,\Big(\gamma\delta\,(1-p)^2+(1-p)\,(p\,(\gamma+\delta)-(\delta\alpha+\beta\gamma))-p\,((1-\alpha)\,\beta+\alpha-p)\Big)\\ &+p^2q^2\,\Big(\alpha\,\gamma\,\left((1-\delta)^2-(1-\beta)^2\right)+\beta\,\delta\,\left((1-\gamma)^2-(1-\alpha)^2\right)\Big)\\ &+p^2q^3\,\Big(\beta\,\delta\,(1-\alpha)^2+\alpha\,\gamma\,(1-\beta)^2-\gamma\,\delta\,(1-\alpha)\,(1-\beta)\Big)\\ &-p^3q^2\,\Big(\alpha\,\gamma\,(1-\delta)^2+\beta\,\delta\,(1-\gamma)^2-\alpha\,\beta\,(1-\gamma)\,(1-\delta)\Big)\\ &+p^2q^2\,\left(q^2\gamma\,\delta\,(1-\alpha)\,(1-\beta)-p^2\alpha\,\beta\,(1-\gamma)\,(1-\delta)\right)\qquad=0\,.\end{aligned} \tag{3.9}$$

This is the condition for the existence of a two-dimensional matrix-product state. Like (3.2) this condition is symmetric under the exchange of p with q, α with δ and β with γ.

To specify the two-dimensional representation completely one has to determine the boundary vectors $\langle W|$ and $|V\rangle$ that belong to the solution (3.6), (3.8) and (3.9). They are straightforwardly obtained by determining the nullspaces of the matrices in (3.7):

$$\begin{aligned}|V\rangle&=\begin{pmatrix}(\beta+\delta)\,(\mathcal{A}(p-q)+1-p)\\ \mathcal{A}^2\,(1-\delta-\beta)\,(p-q)-\mathcal{A}\,(p-q+(1-p)\,\delta+\beta\,(1+q-2\,p))+\beta\,(1-p)\end{pmatrix}\,,\\ |W\rangle&=\begin{pmatrix}(1-\mathcal{A})\left\{\mathcal{A}\,(p-q)\,(pq-\gamma p\,(1-p)-\alpha q\,(1-q))+\gamma p^2\,(1-p)\right\}-\mathcal{A}\alpha q^2\,(1-q)\\ pq\,(\alpha+\gamma)\,(\mathcal{A}(p-q)+1-p)\end{pmatrix}.\end{aligned} \tag{3.10}$$

Inserting herein (3.8) one can check that $\langle W|V\rangle$ is neither zero nor singular on the manifold given by (3.9). In passing we note that the case of symmetric diffusion in the bulk of the chain ($q=p$) is not permitted because in this case the normalization vanishes, i.e. $\langle W|V\rangle=0$.

In order to illustrate the meaning of (3.9) we are now going to look at a few special cases of it. Firstly, consider deterministic hopping exclusively to the right, i.e. $p=1$ and $q=0$. One observes that in this special case the condition (3.9) is satisfied automatically, indicating that one can find a two-dimensional representation for arbitrary boundary probabilities α, β, γ, δ if the bulk rates are $p=1$, $q=0$. This is consistent with [9] where a two-dimensional representation was written down at $p=1$, $q=\gamma=\delta=0$ and arbitrary probabilities α and β. However, it should be noted that we may not directly set $p=1$ in our solution, because then one finds $\mathcal{A}=0$ from (3.8) and singularities appear in (3.6).

Another interesting case is obtained when $\gamma = \delta = 0$, but $p \neq 0$, $\alpha \neq 0 \neq \beta$. Here (3.9) simplifies considerably:

$$(1-q)\{(1-p-q)\alpha\beta + q(\alpha+\beta)\} = q(p-q)\,. \tag{3.11}$$

This is a hyperbola in the α-β-plane which intersects the axes at $(p-q)/(1-q)$.

A final case of particular interest is the Hamiltonian limit. This limit of the condition (3.9) is obtained by inserting (2.7) and keeping only the leading order in ρ. Like in the case of a one-dimensional representation we recover the known result, namely eq. (81) of [19].

One might think that the condition (3.9) arises from the special mechanism (2.4) and (2.5). However, for $\gamma = \delta = 0$ we have checked that the solution obtained above is the most general two-dimensional one in the following sense: As mentioned at the end of the discussion of the scalar product state one eliminates the alternating structure in space by introducing a four-state model that uses block-spin variables for two neighbouring sites. Then one can make a homogenous matrix-product ansatz with four independent operators for each two-site block. One further requires the matrix representation of the operators to be independent of the chain length N. Then already a comparison with the groundstate of the transfer matrix T at $N \in \{2,4,6\}$ leads to the condition (3.11).

There also exist representations where $C = \widehat{C}$ is not diagonalizable. We do not discuss them explicitly here because we are not going to make use of them in the sequel. The interested reader may find some results in appendix A. We mention that non-trivial Jordan forms give rise to power laws with positive exponents in the correlation functions (see e.g. [8]), in particular for two-dimensional matrices to a density profile that is linear in space. Physically, this is related to phase transitions in the system.

Finally, we turn to the question that was one of our motivations for constructing the above matrix-product state, namely how the state given by (3.6), (3.8) – (3.10) behaves in the sequential limit. First one observes that the matrices (3.6) have the property

$$A - \widehat{A} = \widehat{B} - B = \frac{\mathcal{A}(1-\mathcal{A})(p-q)}{1-p+(p-q)\mathcal{A}}\mathbb{1} = g(p,q;\alpha,\beta,\gamma,\delta)\mathbb{1}\,. \tag{3.12}$$

The function g is obtained by inserting (3.8) and too complicated to be presented here. Obviously, an analogous results holds also for the one-dimensional case because the difference of any two numbers trivially is a multiple of the identity.

Having observed the property (3.12) for the two-dimensional representation, it is natural to restrict one's attention to those representations of the algebra (2.6) where $A - \widehat{A}$ and $\widehat{B} - B$ are represented by the same multiple of the identity. As we will see soon, such a condition enables one to make full use of the machinery developed for the algebra (2.12) in [18] and [19].

However, let us for the moment concentrate on the one- and two-dimensional representations. Using (3.12) to eliminate e.g. $\widehat{A}$ and $\widehat{B}$, the conditions (2.6) turn into

$$\begin{aligned} \langle W|\,(\alpha A - \gamma B) &= g\,\langle W|\,, \\ (\beta B - \delta A)\,|V\rangle &= g\,\left(1-\beta-\delta\right)|V\rangle\,, \\ pBA - qAB &= g\,\left(((1-q)B + (1-p)A\right)\,. \end{aligned} \tag{3.13}$$

This looks already very similar to (2.12). In order to establish the correspondence manifestly, one inserts (2.7) into the two-dimensional representation (3.6), (3.8) – (3.10) and also into (3.13). Then it is straightforward to check that the limits $\rho \to 0$ of all four operators A, B, $\widehat{A}$, $\widehat{B}$ exist and are non-zero. Furthermore, one finds that $\widehat{A} \to A$ and $\widehat{B} \to B$ as is to be expected because the alternating sublattice structure must vanish in the sequential limit. The boundary vectors with the normalization as in (3.10) have the property $|V\rangle = \rho\left(|V^{(0)}\rangle + \mathcal{O}(\rho)\right)$ and $|W\rangle = \rho^3\left(|W^{(0)}\rangle + \mathcal{O}(\rho)\right)$ with non-vanishing vectors $|V^{(0)}\rangle$ and $|W^{(0)}\rangle$. Finally, the function g appearing in (3.13) behaves as $g(p,q;\alpha,\beta,\gamma,\delta) = \rho\,\widetilde{g}(\widehat{p},\widehat{q};\widehat{\alpha},\widehat{\beta},\widehat{\gamma},\widehat{\delta}) + \mathcal{O}(\rho^2)$ with a non-vanishing function $\widetilde{g}$ of the rates in the sequential limit. Now one inserts all this into (3.13) and keeps only the leading orders in ρ. Identifying finally $\lim_{\rho\to 0} A =: \widetilde{g}\,E$ and $\lim_{\rho\to 0} B =: \widetilde{g}\,D$ one recovers precisely (2.12). Thus, we have shown for the one- and two-dimensional representations constructed above that the matrix-product mechanism (2.4), (2.5) leads precisely to the known mechanism (2.10), (2.11) in the sequential limit. The crucial step to this end was the observation (3.12).

4. Physical quantities from the representations

In this Section we present results for quantities of physical interest such as the bulk density, the current and the correlation length. The computations are based on the one- and two-dimensional representation of the previous Section. In order to present the results in a compact form it will be convenient to introduce an abbreviation which (as we will explain in more detail later) is related to the variables $\kappa_\pm$ used in [18, 19]:

$$\widetilde{\kappa}_\pm(x,y) = \frac{1}{2x}\Big(-x(1-q) + y(1-p) + p - q \\ \pm \sqrt{\left(-x(1-q)+y(1-p)+p-q\right)^2 + 4xy\,(1-q)\,(1-p)}\Big)\,, \tag{4.1}$$

where either α and γ or β and δ will be substituted for the arguments x and y. To understand the meaning of this quantity consider the special case $\gamma = \delta = 0$. First one notes that $\widetilde{\kappa}_+(x,0) = -(1-q) + (p-q)/x$ and $\widetilde{\kappa}_-(x,0) = 0$. Thus, for $p \neq q$ and zero boundary probability y, the expression $\widetilde{\kappa}_+(x,0)$ is basically the inverse of the probability x whereas $\widetilde{\kappa}_-(x,0)$ is trivial. Turning on $y > 0$ means that one not only injects particles e.g. at the left boundary but also extracts them again. Now the variables $\widetilde{\kappa}_+(x,y)$ can be thought of as effective particle input and output rates. They are non-trivial because particles can be e.g. injected at the left boundary, then diffuse some time in the interior before they return to the left boundary where they are then extracted again. If this interpretation of the $\widetilde{\kappa}_+(x,y)$ is correct, they should be related to the ratio of x and y if hopping in the bulk is sufficiently suppressed. Indeed, in the limit $p \to 0$, $q \to 0$ one finds from (4.1) that $\widetilde{\kappa}_+(x,y) \to y/x$.

It should be noted that wherever the abbreviations $\widetilde{\kappa}_\pm$ are used one has to be careful with the range of validity of the result due to the ambiguity of the sign of the square root in (4.1). In order to be on safe grounds we restrict to $p > q$. The results for the case $p < q$ can be recovered using parity, i.e. by exchanging p with q, α with δ and β with γ.

Now we turn to the computation of physical quantities. We shall be interested only in the thermodynamic limit $N \to \infty$. In this limit, the computation amounts to taking

appropriate matrix elements of the relevant operators as the following argument shows. Let $C_{i,i}$ be the largest of the diagonal matrix elements of C. Then in $C^n|V\rangle$ and in $\langle W|C^m$ the ith basis vector in the auxiliary space will yield the dominant contribution if n respectively m is large. Thus, only the ith matrix elements of the operators corresponding to the quantities of interest will contribute in the thermodynamic limit. Below, we will refrain from presenting results that are obtained immediately by inserting the matrix elements of the one- and two-dimensional representations, but will instead present a formulation using the $\widetilde{\kappa}_\pm$ that we have just introduced. These variables are used because we believe that the results given in terms of them will be valid also off the manifolds in the phase diagram accessible by the one- and two-dimensional representations (see also Section 6).

We first compute the density profile which is given by $\langle\tau_x\rangle = \langle W|C^{x-1}BC^{N-x}|V\rangle / \langle W|C^N|V\rangle$ for x odd and by $\langle\widehat{\tau}_x\rangle = \langle W|C^{x-1}\widehat{B}C^{N-x}|V\rangle/\langle W|C^N|V\rangle$ for x even. These profiles are independent of x for any scalar product state. Their values can be written down immediately for the product state (3.1). The only non-trivial computation is to show that the resulting expressions are equivalent to

$$\langle\tau_x\rangle = \frac{\widetilde{\kappa}_+(\beta,\delta)}{1-q+\widetilde{\kappa}_+(\beta,\delta)}\,, \qquad \langle\widehat{\tau}_x\rangle = \frac{\widetilde{\kappa}_+(\beta,\delta)}{1-p+\widetilde{\kappa}_+(\beta,\delta)} \tag{4.2a}$$

and also to

$$\langle\tau_x\rangle = \frac{1-p}{1-p+\widetilde{\kappa}_+(\alpha,\gamma)}\,, \qquad \langle\widehat{\tau}_x\rangle = \frac{1-q}{1-q+\widetilde{\kappa}_+(\alpha,\gamma)} \tag{4.2b}$$

on the manifold given by (3.2).

For the two-dimensional representation (3.6), (3.8) and (3.10), the density profiles depend on the spatial variable x. However, in the bulk of the system, the densities become constant and follow easily from the observation made above: $\langle\tau_x\rangle \approx B_{i,i}/C_{i,i}$ and $\langle\widehat{\tau}_x\rangle \approx \widehat{B}_{i,i}/C_{i,i}$ for $1 \ll x \ll N$. For the two-dimensional representation (3.6) and (3.8) two cases have to be distinguished: $C_{2,2} > C_{1,1}$ which we denote by 'I' and $C_{1,1} > C_{2,2}$ which we denote by 'II'. This corresponds to two different regions in the phase diagram, see Fig. 3 below.

The results obtained from the two-dimensional representation for the bulk ($1 \ll x \ll N$) can be identified with the result (4.2) on the manifold given by (3.9). One finds that (4.2a) is valid in case I and (4.2b) applies to case II. Note that we recover the result for sequential dynamics (eq. (100) of [19]) in the limit of small hopping probabilities. Like in [19] we regard the fact that we obtain the same result from the one- and two-dimensional representations as an indication that the expressions (4.2) may be valid throughout the corresponding phases. For the special case $\gamma = \delta = 0$ they simplify to

$$\langle\tau_x\rangle = 1-\beta\frac{1-q}{p-q}\,, \qquad \langle\widehat{\tau}_x\rangle = \frac{1}{1-\beta}\langle\tau_x\rangle\,, \tag{4.3a}$$

$$\langle\tau_x\rangle = \frac{\alpha}{1-\alpha}\,\frac{1-p}{p-q}\,, \qquad \langle\widehat{\tau}_x\rangle = (1-\alpha)\langle\tau_x\rangle + \alpha\,, \tag{4.3b}$$

for case I or II, respectively.

Next we discuss the current. The current can be computed in the interior of the system at those places where hopping processes are possible during the next time step and is given by expectation values of the operator

$$\widehat{J} = p\widehat{B}A - q\widehat{A}B\,. \tag{4.4}$$

During the first time step it can also be computed at the boundaries where it is given by expectation values of the operators $\widehat{J}_L = \alpha A - \gamma B$ and $\widehat{J}_R = \beta\widehat{B} - \delta\widehat{A}$ respectively.

First, we use this to compute the current from the scalar product state (3.1). The result obtained directly from (3.1) can be written on the manifold (3.2) either as

$$J = \beta \frac{(p-q) - (\beta+\delta)(1-q+\widetilde{\kappa}_-(\beta,\delta))}{(p-q)\,(1-\beta-\delta)}\,, \tag{4.5a}$$

or as

$$J = \alpha \frac{(p-q) - (\alpha+\gamma)(1-q+\widetilde{\kappa}_-(\alpha,\gamma))}{(p-q)\,(1-\alpha-\gamma)}\,. \tag{4.5b}$$

It is easy to specialize this result to $\gamma = \delta = 0$ after recalling that $\widetilde{\kappa}_-(x,0) = 0$. In this special case e.g. (4.5a) turns into $J = \beta\,\frac{(p-q)-\beta(1-q)}{(p-q)(1-\beta)}$.

Analogously the current can be computed from the two-dimensional representation. In order to obtain the result for the thermodynamic limit one now has to compute it by taking the matrix elements $J_L = \left(\alpha\langle W|A - \gamma\langle W|B\right)_i / \left(\langle W|C\right)_i$ at the left boundary, $J_R = \left(\beta\widehat{B}|V\rangle - \delta\widehat{A}|V\rangle\right)_i / \left(C|V\rangle\right)_i$ at the right boundary and $J = \left(p\widehat{B}A - q\widehat{A}B\right)_{i,i} / C^2_{i,i}$ in the interior where i is chosen such that $C_{i,i}$ is maximal. Inserting (3.6), (3.8) and (3.10) here, one finds the simplest result at the left boundary for $i = 1$. The current is equal to (4.5a) in case I and to (4.5b) in case II on the manifold where (3.9) is valid. In the limit of small probabilities this result goes into the one obtained for sequential dynamics, namely eqs. (4.10) and (4.11) of [18]. It is not a coincidence that we have obtained the same expressions for the current from the one- and two-dimensional representations, because (as we will show in the Section 6) they are valid throughout the corresponding phases.

Finally, we turn to the correlation length ζ for the two-dimensional representation which is related to the eigenvalues of C via $\exp(1/\zeta) = C_{2,2}/C_{1,1}$. It is given by

$$\exp\left(\frac{1}{\zeta}\right) = \frac{\widetilde{\kappa}_+(\alpha,\gamma)\,(1-p+\widetilde{\kappa}_+(\beta,\delta))\,(1-q+\widetilde{\kappa}_+(\beta,\delta))}{\widetilde{\kappa}_+(\beta,\delta)\,(1-p+\widetilde{\kappa}_+(\alpha,\gamma))\,(1-q+\widetilde{\kappa}_+(\alpha,\gamma))} \tag{4.6}$$

on the manifold (3.9). To be precise, we have been able to establish the validity of (4.6) analytically for either $\gamma = 0$ or $\delta = 0$. For both rates non-zero we have performed a careful numerical verification. As expected, the result of [19] (eq. (102) loc. cit.) is recovered in the limit of small probabilities. Whether (4.6) is also valid off the manifold specified by (3.9), and if so, in which areas, is beyond the scope of this paper.

The result (4.6) can also be used to translate the inequalities between $C_{2,2}$ and $C_{1,1}$ into inequalities between $\widetilde{\kappa}_+(\alpha,\gamma)$ and $\widetilde{\kappa}_+(\beta,\delta)$. On the manifold (3.9) one finds numerically that $\widetilde{\kappa}_+(\alpha,\gamma)\widetilde{\kappa}_+(\beta,\delta) > (1-p)(1-q)$ [2]). This can be used to infer from (4.6) that $C_{2,2} > C_{1,1}$ (case I) iff $\widetilde{\kappa}_+(\beta,\delta) > \widetilde{\kappa}_+(\alpha,\gamma)$ and vice versa.

[2]) According to [19] one expects that $\widetilde{\kappa}_+(\alpha,\gamma)\widetilde{\kappa}_+(\beta,\delta) \geq (1-p)(1-q)$ holds for any finite-dimensional representation whereof infinitely many should exist. This inequality can be obtained by applying the argument of the next Section to the corresponding inequality of [19].

5. Mapping onto the Hamiltonian limit

In this Section we will impose a condition similar to (3.12) for general values of the parameters and use this to map the problem for parallel dynamics to the one with sequential dynamics.

After fixing the normalization of the representation of the operators A, B, $\widehat{A}$ and $\widehat{B}$ suitably (but different from the one used in Section 3), we will from now on concentrate on representations where

$$\widehat{B} - B = A - \widehat{A} = \mathbb{1} \tag{5.1}$$

holds (this condition has also been proposed in [14]). This choice may be a restriction in the sense that representations of the algebra (2.6) might exist that are not equivalent to one where (5.1) holds. We will now show that (5.1) can be used to lift the Fock space representation of the algebra (2.12) to a representation of the algebra (2.6) and therefore one can (at least in principle) compute stationary expectation values for arbitrary probabilities α, β, γ, δ, p and q. Even if other representations of the parallel algebra should exist, they would have to give rise to the same groundstate that can also be obtained from a representation where (5.1) is valid. Thus, from a physical point of view it is completely sufficient to study only representations satisfying (5.1).

We attempt a mapping to the sequential algebra (2.12) by identifying E with a suitable linear combination of A and $\widehat{A}$ and D with another suitable linear combination of B and $\widehat{B}$. This leads to the following ansatz for the operators A, $\widehat{A}$, B and $\widehat{B}$ in terms of E and D:

$$\begin{aligned} A &= n_E E + e\mathbb{1}\,, \qquad & \widehat{A} &= n_E E - (1-e)\mathbb{1}\,, \\ B &= n_D D - d\mathbb{1}\,, \qquad & \widehat{B} &= n_D D + (1-d)\mathbb{1}\,, \end{aligned} \tag{5.2}$$

where the free constants n_E and n_D reflect the freedom of choice of relative normalization of the representations and the constants e and d correspond to the points of identification. Inserting this ansatz into (2.6a) one obtains precisely one independent relation between E and D:

$$\begin{aligned} n_E n_D (pDE - qED) =& n_E E\,(d(p-q) + (1-p)) + n_D D\,(-e(p-q) + (1-q)) \\ &+ ed(p-q) + e(1-p) - d(1-q)\,. \end{aligned} \tag{5.3}$$

In order to be able to identify this with (2.12) the constant term in (5.3) must vanish. This is ensured by chosing

$$e = \frac{d(1-q)}{d(p-q) + (1-p)}\,. \tag{5.4}$$

Also the linear term in E must appear with the same coefficient as the linear term in D on the r.h.s. of (5.3). This is the case if

$$n_D = -n_E \frac{d(p-q) + (1-p)}{e(p-q) - (1-q)} = n_E \frac{(d(p-q) + (1-p))^2}{(1-p)(1-q)}\,. \tag{5.5}$$

Using (5.4) and (5.5) the relation (5.3) now reads

$$n_E \frac{d(p-q) + (1-p)}{(1-p)(1-q)}\,(pDE - qED) = E + D\,. \tag{5.6}$$

Inserting the ansatz (5.2) into the boundary equations (2.6b) leads to

$$\langle W|\frac{\alpha n_E E - \gamma n_D D}{1-\alpha e - \gamma d} = \langle W|\,, \qquad \frac{\beta n_D D - \delta n_E E}{1+\delta e + \beta d - (\delta+\beta)}|V\rangle = |V\rangle\,. \tag{5.7}$$

The equations (5.6) and (5.7) are identical to the algebra of the sequential limit (2.12) if one identifies the rates in that limit as follows

$$\begin{aligned}
\widehat{p} &= n_E \frac{d(p-q)+(1-p)}{(1-p)(1-q)} p\,, & \widehat{q} &= n_E \frac{d(p-q)+(1-p)}{(1-p)(1-q)} q\,, \\
\widehat{\alpha} &= n_E \frac{1}{1-\alpha e - \gamma d}\alpha\,, & \widehat{\beta} &= n_D \frac{1}{1+\delta e + \beta d - (\delta+\beta)}\beta\,, \\
\widehat{\gamma} &= n_D \frac{1}{1-\alpha e - \gamma d}\gamma\,, & \widehat{\delta} &= n_E \frac{1}{1+\delta e + \beta d - (\delta+\beta)}\delta\,.
\end{aligned} \tag{5.8}$$

Here, the constants e and n_D are fixed by (5.4) and (5.5). The constant n_E remains free and reflects the freedom of normalization of the algebra in the sequential limit. It is possible to choose n_E such that the 'renormalized' rates in the bulk are equal to the hopping probabilities, i.e. $\widehat{p} = p$ and $\widehat{q} = q$. If one does not fix n_E in a computation of a physical quantity, it has to disappear from the final result. Also the constant d is still free in (5.8), but for explicit computations it will, in contrast to n_E, be fixed to a convenient value that ensures $n_E = n_D$. Then, the operators C for the parallel and sequential case may be identified with each other.

From (5.8) one sees that in the sequential limit the renormalized parameters differ from the initial probabilities only by a factor n_E, which also equals n_D because of (5.5). Therefore, choosing $n_E = 1$, both sets of parameters and also the matrix-product states become identical.

One can also check that the conditions of Section 3 for having a one- or two-dimensional representation can be recovered from known results. All one has to do is insert (5.8) where n_E and d are kept as free parameters into the conditions for the sequential limit [19]. The d-independent factors of these renormalized conditions are precisely (3.2) and (3.9) respectively. So, the simple scalar product state as well as the two-dimensional matrix-product state of the general case can be obtained by a simple 'renormalization' process from the ones of the sequential limit. The same holds also for higher-dimensional representations whose existence was shown in [19].

6. Current and phase diagram

Now we show how to use the mapping of the previous Section to compute quantities of physical interest.

According to [18, 19], the phase diagram in the sequential case is given by a single function κ_+ of the rates at either boundary, i.e. by $\kappa_+(\widehat{\alpha},\widehat{\gamma})$ and $\kappa_+(\widehat{\beta},\widehat{\delta})$. The same will hold in parallel case, if the quantities (5.8) are inserted into the functions κ_+. This statement has already been partially verified in Section 4 where the variables $\widetilde{\kappa}_\pm(x,y)$ have been used. To be more precise, the parallel case will be descibed by functions $\widehat{\kappa}_\pm(\alpha,\gamma) = \kappa_\pm(\widehat{\alpha},\widehat{\gamma})$ and $\widehat{\kappa}_\pm(\beta,\delta) = \kappa_\pm(\widehat{\beta},\widehat{\delta})$ which are obtained from the $\kappa_\pm$ of the sequential case [18, 19] by

choosing the constant d in the mapping (5.8) such that $n_D = n_E$. The function $\widehat{\kappa}_\pm$ is given by

$$\widehat{\kappa}_\pm(x,y) = \frac{\widetilde{\kappa}_\pm(x,y)}{\sqrt{(1-q)\,(1-p)}}\,, \tag{6.1}$$

where $\widetilde{\kappa}_\pm(x,y)$ was defined in (4.1). Recall from the beginning of Section 4 that $\widehat{\kappa}_+(\alpha,\gamma)$ and $\widehat{\kappa}_+(\beta,\delta)$ may be regarded as effective input/output rates at the boundaries. Recall also that the $\widetilde{\kappa}_\pm$ and $\widehat{\kappa}_\pm$ should be used only for $p > q$ and that the results for the case $p < q$ can be obtained by applying parity.

It is straightforward to compute the currents for the general case with parallel dynamics using the results of [18] for the sequential case. The operators needed for that have already been given in (4.4) for the bulk and for the boundaries below that equation. Using (2.6b) and the ansatz (5.1) one can check that

$$\begin{aligned} J_L &= \frac{\langle W|\,(\alpha A - \gamma B)\,C^{N-1}|V\rangle}{\langle W|C^N|V\rangle} = \frac{\langle W|C^{N-1}|V\rangle}{\langle W|C^N|V\rangle} = J \\ &= \frac{\langle W|C^{N-1}\left(\beta\widehat{B} - \delta\widehat{A}\right)|V\rangle}{\langle W|C^N|V\rangle} = J_R\,. \end{aligned} \tag{6.2}$$

This means that the current is simply given by ratios of the normalization constants $\langle W|C^N|V\rangle$ for different N if the condition (5.1) holds. Thus, in order to compute the current in the thermodynamic limit, the behaviour of such ratios has to be studied for large N.

One finds from (5.2) that

$$C = A + B = n_E(E + D) + (e - d)\,. \tag{6.3}$$

In [18] the operators D and E have been expressed in terms of the creation and annihilation operators F and $F^\dagger$ of a q-deformed harmonic oscillator by setting

$$D = \frac{F+1}{\widehat{p}-\widehat{q}}\,, \qquad E = \frac{F^\dagger+1}{\widehat{p}-\widehat{q}}\,. \tag{6.4}$$

Inserting this into (6.3) leads to

$$C = n_E\frac{F + F^\dagger + \lambda}{\widehat{p}-\widehat{q}} \tag{6.5}$$

with

$$\lambda = 2 + (e-d)\frac{\widehat{p}-\widehat{q}}{n_E} = \frac{2-q-p}{\sqrt{(1-q)(1-p)}}\,. \tag{6.6}$$

First we consider the case $\widehat{\kappa}_+(\alpha,\gamma) < 1$ and $\widehat{\kappa}_+(\beta,\delta) < 1$. According to [18] this is the maximal current phase and to obtain J, the same computation as there can be used. In eq. (3.39) loc. cit. the coefficient 2 of c^L_{ik} has to be replaced by λ because of the extra constant

in (6.5). Tracing the effect of this modification one finds that for parallel dynamics the current in the maximal current phase is given by

$$J = \frac{1}{n_E}\,\frac{\widehat{p}-\widehat{q}}{2+\lambda} = \frac{\sqrt{1-q}-\sqrt{1-p}}{\sqrt{1-q}+\sqrt{1-p}}\,. \tag{6.7}$$

For small p and q the result (4.6) of [18] is recovered.

This result can be checked [21] using the one-dimensional representation because the line (3.2) touches the region where (6.7) is valid (see Fig. 3 below).

The currents for the other two phases can be obtained from similar modifications of the computations in [18]. First we consider the case $\widehat{\kappa}_+(\beta,\delta) > \widehat{\kappa}_+(\alpha,\gamma)$ and $\widehat{\kappa}_+(\beta,\delta) > 1$. The relation (4.7) of [18] remains valid with the new parameters and reads

$$\langle W|C^{N-1}F|V\rangle \approx \kappa_+(\widehat{\beta},\widehat{\delta})\langle W|C^{N-1}|V\rangle = \widehat{\kappa}_+(\beta,\delta)\langle W|C^{N-1}|V\rangle\,. \tag{6.8}$$

One can further rewrite C as follows using (6.3) – (6.6)

$$\begin{aligned} C =& \frac{n_E}{\widehat{\delta}}\left(-(\widehat{\beta}D-\widehat{\delta}E) + \frac{\widehat{\beta}+\widehat{\delta}+\widehat{\delta}\,(\widehat{p}-\widehat{q})(e-d)/n_E}{\widehat{p}-\widehat{q}} + \frac{\widehat{\beta}+\widehat{\delta}}{\widehat{p}-\widehat{q}}F\right) \\ =& \frac{n_E}{\widehat{\delta}}\left(-(\widehat{\beta}D-\widehat{\delta}E) + \frac{\widehat{\beta}+\widehat{\delta}+\widehat{\delta}(\lambda-2)}{\widehat{p}-\widehat{q}} + \frac{\widehat{\beta}+\widehat{\delta}}{\widehat{p}-\widehat{q}}F\right)\,. \end{aligned} \tag{6.9}$$

Making first use of (6.9) and then of (6.8) one finds the following recurrence relation for the normalization constants (generalizing eqs. (4.8) and (4.9) of [18])

$$\begin{aligned} &\langle W|C^N|V\rangle \\ &= \frac{n_E}{\widehat{\delta}}\,\frac{1}{\widehat{p}-\widehat{q}}\left\{\left(\widehat{\beta}+\widehat{\delta}+\widehat{\delta}(\lambda-2)-\widehat{p}+\widehat{q}\right)\langle W|C^{N-1}|V\rangle + \left(\widehat{\beta}+\widehat{\delta}\right)\langle W|C^{N-1}F|V\rangle\right\} \\ &\approx \frac{n_E}{\widehat{\delta}}\,\frac{1}{\widehat{p}-\widehat{q}}\left\{\left(\widehat{\beta}+\widehat{\delta}+\widehat{\delta}(\lambda-2)-\widehat{p}+\widehat{q}\right) + \left(\widehat{\beta}+\widehat{\delta}\right)\widehat{\kappa}_+(\beta,\delta)\right\}\langle W|C^{N-1}|V\rangle\,. \end{aligned} \tag{6.10}$$

Inserting this result into (6.2) one recovers after a straightforward computation the result (4.5a) that we already obtained from the one- and two-dimensional representations. The result for the other phase $\widehat{\kappa}_+(\alpha,\gamma) > \widehat{\kappa}_+(\beta,\delta)$ and $\widehat{\kappa}_+(\alpha,\gamma) > 1$ can be obtained simply by replacing β by α and δ by γ and coincides with (4.5b).

These results can be used to draw the phase diagram which turns out to be essentially the same as the one for the sequential limit [18, 19]. It is shown in Fig. 3 in terms of the variables $\widehat{\kappa}_+(x,y)$, using a logarithmic scale. There are at least three distinct phases which are characterized only by the values of $\widehat{\kappa}_+(\alpha,\gamma)$ and $\widehat{\kappa}_+(\beta,\delta)$:

I: $\widehat{\kappa}_+(\beta,\delta) > \widehat{\kappa}_+(\alpha,\gamma)$, $\widehat{\kappa}_+(\beta,\delta) > 1$ (high density)
II: $\widehat{\kappa}_+(\alpha,\gamma) > \widehat{\kappa}_+(\beta,\delta)$, $\widehat{\kappa}_+(\alpha,\gamma) > 1$ (low density)
III: $\widehat{\kappa}_+(\alpha,\gamma) < 1$, $\widehat{\kappa}_+(\beta,\delta) < 1$ (maximal current)

The density in phases I and II is approximately constant in the bulk. On the coexistence line $\widehat{\kappa}_+(\alpha,\gamma) = \widehat{\kappa}_+(\beta,\delta)$ which separates these two phases the density profile is linear in space.

Phases I and II can be mapped onto each other using parity and particle-hole symmetry. This 'duality' transformation exchanges $\tau_x \leftrightarrow 1 - \widehat{\tau}_{N+1-x}$, $\alpha \leftrightarrow \beta$, $\gamma \leftrightarrow \delta$ and keeps p and q unchanged. In particular $\widehat{\kappa}_+(\alpha,\gamma)$ is exchanged with $\widehat{\kappa}_+(\beta,\delta)$ from which one obtains the mapping between the two phases.

The dotted line in Fig. 3 shows the condition (3.2) for the existence of a one-dimensional representation which can be cast in the form $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) = 1$. The figure also shows the condition (3.9) for having a two-dimensional representation with two choices of p and q. In both cases $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) = p/q$ is verified numerically. For $\gamma = \delta = 0$, it can also be shown analytically that this condition is equivalent to (3.9). This suggests that the condition for having a two-dimensional representation is a hyperbola in the $\widehat{\kappa}_+(\alpha,\gamma)$-$\widehat{\kappa}_+(\beta,\delta)$ plane. By changing the value of p/q this hyperbola can be swept over the entire region above the dotted line marking the one-dimensional representation.

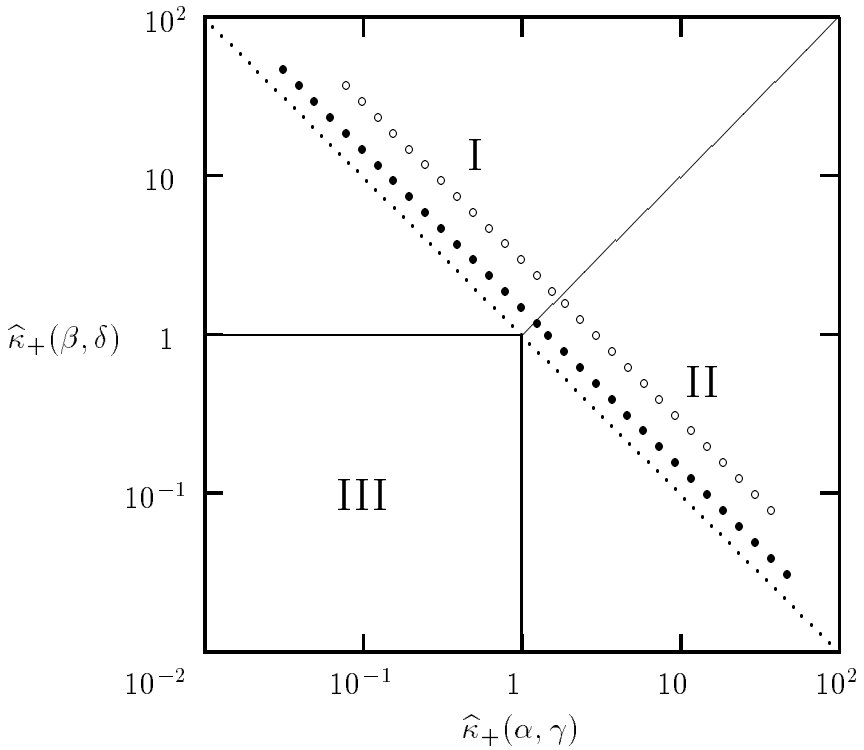


Fig. 3: Phase diagram of the kinetic model. The dotted line shows the condition (3.2) for a one-dimensional representation. The condition (3.9) for a two-dimensional representation is shown for two choices of p and q: The symbol '$\circ$' is for $p = 0.75$, $q = 0.25$ and the symbol '$\bullet$' is for $p = 0.6$, $q = 0.4$.

For a more detailed discussion of the case $\gamma = \delta = 0$ we refer to [21].

Our results for the current and densities are summarized in Table 1. The correlation length is given by (4.6), but probably not throughout the entire phases I and II. Presumably one has to choose at least $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) > 1$ because on the line $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) = 1$ there is a scalar product state and the correlation length diverges as one approaches this line.

All these results have the correct behaviour under the duality transformation which exchanges the phases I and II.

Phase	J	$\langle\tau_x\rangle$	$\langle\widehat{\tau}_x\rangle$
I	$\beta\,\dfrac{(p-q)-(\beta+\delta)(1-q+\widetilde{\kappa}_-(\beta,\delta))}{(p-q)\,(1-\beta-\delta)}$	$\dfrac{\widetilde{\kappa}_+(\beta,\delta)}{1-q+\widetilde{\kappa}_+(\beta,\delta)}$	$\dfrac{\widetilde{\kappa}_+(\beta,\delta)}{1-p+\widetilde{\kappa}_+(\beta,\delta)}$
II	$\alpha\,\dfrac{(p-q)-(\alpha+\gamma)(1-q+\widetilde{\kappa}_-(\alpha,\gamma))}{(p-q)\,(1-\alpha-\gamma)}$	$\dfrac{1-p}{1-p+\widetilde{\kappa}_+(\alpha,\gamma)}$	$\dfrac{1-q}{1-q+\widetilde{\kappa}_+(\alpha,\gamma)}$
III	$\dfrac{\sqrt{1-q}-\sqrt{1-p}}{\sqrt{1-q}+\sqrt{1-p}}$	———	———

Table 1: Summary of our results for the current J, the bulk density $\langle\tau_x\rangle$ on the odd sublattice and the bulk density $\langle\widehat{\tau}_x\rangle$ on the even sublattice in the three phases.

We mention that the result for the current can also be obtained by using the bulk-densities in the mean-field formula $J = p\langle\widehat{\tau}_x\rangle(1-\langle\tau_{x+1}\rangle) - q(1-\langle\widehat{\tau}_x\rangle)\langle\tau_{x+1}\rangle$. In regions I and II this can be shown analytically for $\gamma = \delta = 0$. In region III it can be verified numerically.

In appendix B we show how to use (3.12) with $g = 1$ to compute correlation functions for the case of symmetric diffusion $p = q$ where the results of this Section and Section 4 may not be applied directly (compare also the corresponding remark in Section 3). For this special case, the algebra is much simpler. Appendix C describes how one can use the same representation to compute physical quantities on finite lattices with system sizes up to a few hundred sites. This can be used to check the validity of our results in Table 1 as well as the correlation length (4.6) for $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) > 1$ numerically.

7. Discussion

We have considered the diffusion of hard-core particles between two reservoirs for a particular kind of parallel dynamics. The results show that the stationary state has a similar matrix-product form as in the sequential case and can actually be obtained from that limit. Therefore the physical properties, in particular the phase diagram, are also similar although the formulae are more involved.

In [14] it was found that the same is true for yet another type of dynamics, where the stochastic motion takes place step-by-step along the chain. This can be visualized nicely in the vertex-model picture as shown in Fig. 4. The processes take place in a diagonal strip of the lattice and the time-evolution operator is seen to be the usual row-to-row transfer matrix T_{row} of the vertex model, with a shift in the numbering of the upper row of variables and additional boundary vertices. Using the same exchange mechanism at each vertex as in Section 2, one finds that the pair of operators A and B only appears in the intermediate steps and the matrix-product state becomes a homogenous state involving only the operators $\widehat{A}$ and $\widehat{B}$. An independent treatment of this matrix-product state would involve computations similar to those that we have presented here. Alternatively, one can also directly use our results for the current and correlation length for the updates as in Fig. 4 (the densities are only the same on the even sublattice) [14].

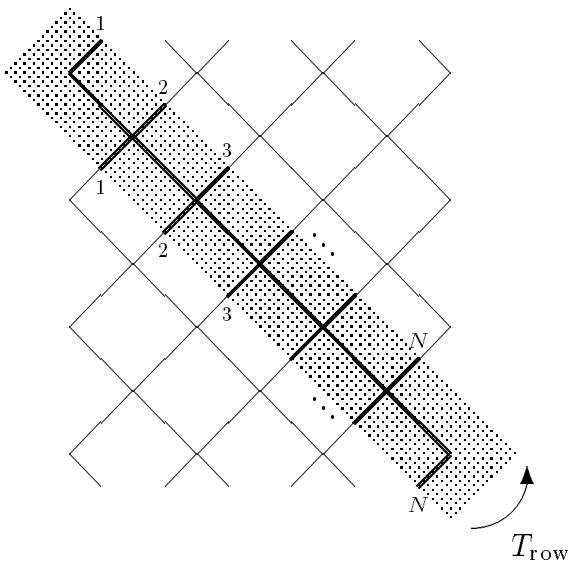
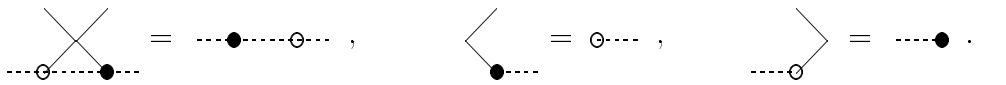


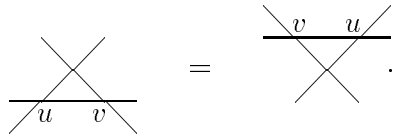
Fig. 4: Representation of a step-by-step dynamics starting at the right end of the system as a vertex model.

In order to illustrate the connection to vertex models further, let us also present a graphical representation of the matrix-product mechanism used here. Denote the pair of operators A, B by a '$\bullet$' and the pair $\widehat{A}$ and $\widehat{B}$ by a '$\circ$'. A dotted line between them indicates that their product is to be taken while a termination of the line inside them means that the vectors $\langle W|$ and $|V\rangle$ have to be multiplied from the left and right respectively. Then (2.5) and (2.4) can be depicted as follows (compare also Fig. 3 of [12]):



(7.1)

The first identity is strikingly similar to the Yang-Baxter equation (see e.g. Chapter 2.3 of [22]) which for vertex models reads graphically



(7.2)

In both cases one can 'pull' a line through the vertex and the corresponding quantities exchange places. The boundary Yang-Baxter equations, involving the so-called K-matrices, are more complicated. This leads us to the question of integrability of the model. As already mentioned, the time evolution operator in the sequential limit is a Heisenberg Hamiltonian with boundary fields. It is therefore integrable in the sense that it belongs to a whole family of commuting operators [23, 24]. One would expect that this also holds for the full vertex model. A proof would have to follow the lines of [23 – 25]. In any case, the integrability would be more relevant for the time behaviour of the system than for the stationary state which we determined.

Occasionally, it has been conjectured that there is a connection between the existence of matrix-product states and integrability. However, examples of scalar product states like in [10] show that this cannot be true in general. Nor does the construction in [26] ensure integrability. It amounts to transforming the bulk relation in (7.1) into a commutator as in (7.2) by going over from the eigenvector $|\Phi\rangle$ to the operator $P = |\Phi\rangle\langle\Phi|$. However, this does not help in finding other eigenstates because P is a simple projector whose unique eigenvector with eigenvalue 1 is $|\Phi\rangle$ while a highly degenerate eigenvalue 0 accounts for all other vectors.

Finally, one may ask if the parallel dynamics considered in this work might be used in other related problems. Here, two situations come to mind. One would be a model with coagulation and decoagulation in addition to the hopping processes. With a proper tuning of the parameters, this is a free-fermion problem in the sequential limit [27] and the stationary state has been shown to have a matrix-product form with four-dimensional matrices [8]. As in the present work, there are four matrices involved, two for the homogenous matrix-product state and two in the generalization of the cancellation mechanism (2.10) and (2.11). Indeed, if the mechanism (2.4) and (2.5) should be applicable to more general situations than discussed here, one would in general not expect the differences $A - \widehat{A}$ and $\widehat{B} - B$ to be proportional to the indentity and thus one would find the more general matrix-product mechanism of [8] in the sequential limit. However, the choice $C = \widehat{C}$ is always possible independent of the details of the dynamics. This would lead to a linear relation between the matrices in the sequential limit, but one can check that the four matrices used in [8] are linearly independent. Thus, whether the problem including coagulation and decoagulation admits a matrix-product state also for parallel dynamics, and if so, with which mechanism, remains to be investigated.

The other problem is hopping on a ring with a defect where the rates are modified. Formally, this case is obtained by replacing the product $\mathcal{R} \otimes \mathcal{L}$ of the boundary matrices by a hopping matrix $\widetilde{\mathcal{T}}$. This model has already been solved by a modified Bethe ansatz for the case of unidirectional deterministic motion everywhere except at the defect [28]. For a certain fixed particle density, the stationary state is also expressible in the form of a two-dimensional matrix product [29]. One may speculate that our representation (3.6) of the bulk algebra may help to solve the general model with a defect. In particular, the observation that the differences of the matrices with and without hat are proportional to the identity is a pure bulk property and thus one may hope that techniques like those we have used e.g. in Sections 5 and 6 may be useful also for systems with a defect.

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Appendix A. Representation with Jordan form

In this appendix we briefly discuss a two-dimensional representation where $C = \widehat{C}$ has a non-trivial Jordan form. This case occurs if $C_{2,2} = 1$ and simultaneously $\langle W|V\rangle = 0$ because then the normalization $\langle W|C^N|V\rangle$ of the groundstate vanishes and the representation with diagonal C may not be used any more. We have not been able to fully determine when this happens in (3.6), (3.8) – (3.10), but one can check that it is the case if $\beta = \alpha$ and $\gamma = \delta$. Using these values in (3.9), one then finds that

$$\left(p\alpha^2 - q\delta^2\right)(1-p)(1-q) + pq\left((1-p)(1-\delta)^2 - (1-q)(1-\alpha)^2\right) = 0\,. \tag{A.1}$$

One can choose

$$C = \widehat{C} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \tag{A.2}$$

by suitably fixing the normalization of C and $\widehat{C}$ and the relative normalization of the two basis vectors in the auxiliary space. The further strategy to determine the representation matrices for A und $\widehat{A}$ is now slightly different from the procedure described in Section 3. First one solves the boundary conditions (2.6b) as described below (3.7). With the result of this computation one can then solve the equations (2.6a). This leads to:

$$\begin{aligned} A &= \frac{1}{\mathcal{B}} \begin{pmatrix} q\delta - \delta + p\delta - p & 0 \\ 0 & q\alpha + q\delta - \alpha - q \end{pmatrix}, \\ \widehat{A} &= \frac{1}{\mathcal{B}} \begin{pmatrix} p\delta - \delta + p\alpha - p & 0 \\ 0 & q\alpha - \alpha + p\alpha - q \end{pmatrix}, \end{aligned} \tag{A.3}$$

with

$$\mathcal{B} = (\alpha+\delta)(p+q-1) - (p+q)\,. \tag{A.4}$$

Again, some freedom was used to set $\widehat{A}_{1,2} = 0$ in (A.3). Instead of (3.10) one now has to choose the boundary vectors as follows:

$$\begin{aligned} |V\rangle &= \begin{pmatrix} \alpha\,\mathcal{B} \\ (\alpha+\delta)\left\{(1-\delta)(1-p) - (1-\alpha)(1-q)\right\} \end{pmatrix}, \\ |W\rangle &= \begin{pmatrix} -(\alpha+\delta)\left\{(1-\delta)(1-p) - (1-\alpha)(1-q)\right\} \\ \delta\,\mathcal{B} \end{pmatrix}. \end{aligned} \tag{A.5}$$

One can check that $\langle W|V\rangle$ is neither zero nor singular on the manifold given by (A.1).

A property similar to (3.12) also holds here and has in fact been assumed to simplify the computations.

We should mention that (A.1) is not recovered after inserting the renormalized rates (5.8) into its sequential limit. However, it is argued in Section 6 that the coexistence line has a more general form than just $\beta = \alpha$, $\gamma = \delta$. Thus, the fact that (A.1) does not reproduce itself under renormalization is a hint that one should be able to find two-dimensional representations where C is given by (A.2) under more general conditions than (A.1).

Appendix B. Symmetric diffusion in the bulk

Here we discuss the special case of symmetric diffusion in the bulk, i.e. $p = q$. In this case, which was also considered in [15], it is convenient to work with the operator B and the spatial transfer-matrix C. Inserting the choice (5.1) into (2.6) leads to

$$\begin{aligned} [B, C] &= \frac{1-p}{p} C \,, \\ \langle W| \left(\alpha C - (\alpha+\gamma) B\right) &= \langle W| \,, \qquad \left((\beta+\delta) B - \delta C\right) |V\rangle = (1-\beta-\delta)\, |V\rangle \,. \end{aligned} \tag{B.1}$$

Using these relations one immediately finds by either commuting the B to the right or the left boundary

$$\begin{aligned} \langle W| C^{x-1} B C^{N-x} |V\rangle &= \left(\frac{1-p}{p}(N-x) + \frac{1-\beta-\delta}{\beta+\delta} \right) \langle W| C^{N-1} |V\rangle + \frac{\delta}{\beta+\delta} \langle W| C^N |V\rangle \\ &= \left(-\frac{1-p}{p}(x-1) - \frac{1}{\alpha+\gamma} \right) \langle W| C^{N-1} |V\rangle + \frac{\alpha}{\alpha+\gamma} \langle W| C^N |V\rangle \,. \end{aligned} \tag{B.2}$$

From these two expressions the term $\langle W| C^{N-1} |V\rangle$ can be eliminated yielding the density profile for the odd sites

$$\langle \tau_x \rangle = \frac{\alpha\ (\beta+\delta)\,(N-1) - (\alpha\,\beta - \gamma\,\delta)\,(x-1) + \frac{p}{1-p}\left\{\alpha\ (1-\beta) + \delta\ (1-\alpha)\right\}}{(\alpha+\gamma)\,(\beta+\delta)\,(N-1) + \frac{p}{1-p}\left\{\alpha\ (1-\beta) + \delta\ (1-\alpha) + \gamma\ (1-\delta) + \beta\ (1-\gamma)\right\}} \,. \tag{B.3}$$

A similar computation with $\widehat{B} = B + \mathbb{1}$ yields the profile for the even sites. The expression differs from (B.3) only in the last curly bracket in the numerator which becomes $\{\alpha\ (1-\delta) + \delta\ (1-\gamma)\}$. In the thermodynamic limit $N \to \infty$ this difference between $\langle \tau_x \rangle$ and $\langle \widehat{\tau}_x \rangle$ disappears and, more strikingly, the densities become independent of the bulk probability p. The result after the limit is identical to the one obtained in [30] for the case of sequential updates.

For finite N, the density profile (B.3) is linear in the spatial variable x (as one can already see from (B.2)). For $p = q$ the current is related to the density profile by $J = p\,(\langle \widehat{\tau}_x \rangle - \langle \tau_{x+1} \rangle)$. Inserting the result (B.3) one finds that

$$J \approx p \frac{\alpha\,\beta - \gamma\,\delta}{(1-p)\,(\alpha+\gamma)\,(\beta+\delta)} N^{-1} \tag{B.4}$$

for N large. Physically, this means that the pumping effect at the ends is not sufficient to drive a current through an infinite system. The results (B.3) and (B.4) show that only one phase exists which corresponds to the coexistence line in Fig. 3.

It is straightforward to apply the method used above for computing the density profile also to higher correlation functions.

Although for the case discussed here the groundstate is comparably simple, this is still interesting because for $p = q$ our local bulk-transfer-matrix $\mathcal{T}$ becomes identical to the R-matrix $\check{R}$ of the symmetric six-vertex model. One can parametrize $p = u/(u+\eta)$ where u is the spectral parameter and η a constant. With this parametrization the Yang-Baxter

equation (7.2) with spectral parameter u is satisfied and can be used to write down a family of commuting stochastic row-to-row transfer matrices for periodic boundary conditions (see e.g. Chapter 2.3 of [22]). Thus, the hopping probability p is essentially the spectral parameter of an integrable model. One consequence probably is the disappearance of p from the density profile (B.3) in the thermodynamic limit.

For $p \neq q$, the $\mathcal{T}$-matrices (2.2) can be identified with the $\check{R}$-matrix of the general asymmetric six-vertex model with a suitable spectral parameter u:

$$\check{R} = \begin{pmatrix} \sin(u+\eta) & 0 & 0 & 0 \\ 0 & z^u \sin(\eta) & x \sin(u) & 0 \\ 0 & x^{-1} \sin(u) & z^{-u} \sin(\eta) & 0 \\ 0 & 0 & 0 & \sin(u+\eta) \end{pmatrix}, \tag{B.5}$$

where η, x and z are some arbitrary constants. One can show that this also satisfies the Yang-Baxter equation (7.2). However, the impact of the boundary vertices in Fig. 2 on the integrability remains to be fully clarified.

Appendix C. Computations on finite chains

We show here how to compute correlation functions efficiently using a representation of the algebra where (5.1) holds. Then A and B satisfy (3.13) with $g = 1$. A convenient basis for the Fock space is given by $B^x|V\rangle$ and one then has to compute $AB^x|V\rangle$. In order to describe how this can be done e.g. on a computer let

$$|x\rangle := B^x|V\rangle\,, \qquad |x,y\rangle := B^x A B^y|V\rangle\,. \tag{C.1}$$

The bulk relation in (3.13) (with $g = 1$) can be used to commute an operator A one place to the right which in terms of the above vectors yields the relation

$$|x,y\rangle = \frac{1}{q}\left(p|x+1,y-1\rangle - (1-p)|x,y-1\rangle - (1-q)|x+y\rangle\right) \tag{C.2}$$

for $y > 0$. As soon as the operator A hits the right boundary one can use the second boundary equation in (3.13) with $g = 1$ to replace A by B:

$$|x,0\rangle = \frac{1}{\delta}\left(\beta|x+1\rangle - (1-(\beta+\delta))|x\rangle\right)\,. \tag{C.3}$$

By definition, the algebra acts on the states (C.1) as

$$A|x\rangle = |0,x\rangle\,, \qquad B|x\rangle = |x+1\rangle\,. \tag{C.4}$$

The rules (C.2) – (C.4) are sufficient to express any state $ABAA\ldots|V\rangle$ in terms of the $|x\rangle$ and one does not need the original algebra anymore. In order to be able to compute words (i.e. scalar products with $\langle W|$) a final constant $s_x := \langle W|x\rangle$ is needed. It can be computed by creating an A at the left boundary using the first boundary relation in (3.13) (with $g = 1$). This leads to

$$s_{x+1} = \frac{1}{\gamma}\left(\alpha\langle W|0,x\rangle - s_x\right) \tag{C.5}$$

which amounts to a recurrence relation for the s_x after moving the A to the right boundary using the previous relations. Setting $s_0 = 1$, one is now able to compute the value of any word $\langle W|ABAA\ldots|V\rangle$ exclusively from the rules (C.2) – (C.5).

It is possible to solve these recurrence relations in closed form following the lines of [18]. However, also formulae of the type as in [18] are best evaluated numerically using a recursive procedure. The recipe presented above is sufficient to compute correlation functions numerically on finite chains where a length $N = 100$ is no major problem. However, in order not to do a computation twice, one should store the expansion of the vectors $|x, y\rangle$ in terms of the basis vectors $|x\rangle$. One also needs to be careful with the numerical range because some of the numbers grow exponentially with N, e.g. $\langle W|C^N|V\rangle \approx J^{-N}$ and $|J^{-1}| \geq 1$ can become quite large [3]).

Fig. 5 shows a density profile obtained in this manner on a finite lattice with $N = 200$. The parameters yield $\widehat{\kappa}_+(\alpha, \gamma) = 0.912$ and $\widehat{\kappa}_+(\beta, \delta) = 0.801$ which to corresponds to a point at the top right corner of phase III in Fig. 3. The distinction between the two sublattices is clearly visible, so is the influence of the boundaries. As a byproduct in this computation one finds the current with these parameters for $N = 200$ using (6.2): $J = 0.2690$. This is to be compared to the result $J = 0.2679$ obtained from (6.7) in the thermodynamic limit. Computations like this one provide room for more detailed investigations.

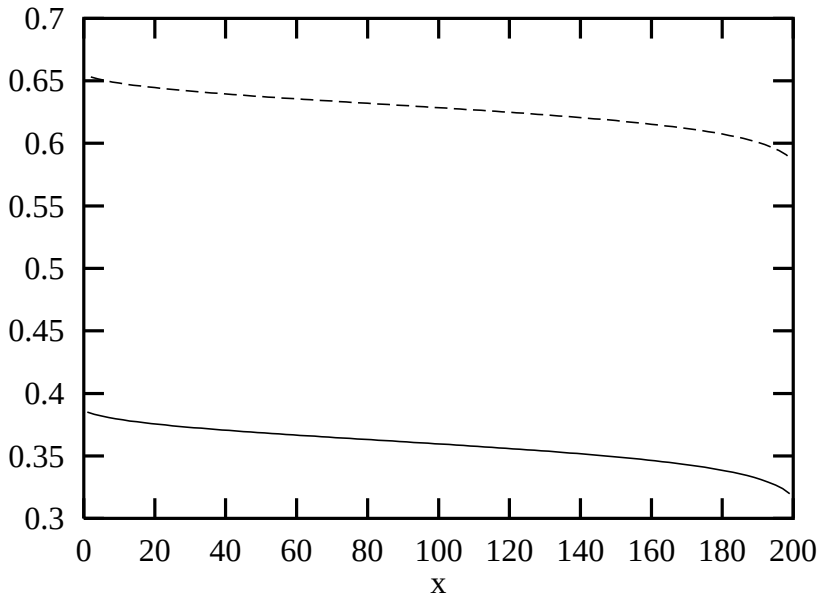

Fig. 5: A density profile in the maximal current phase with $N = 200$ sites and $p = 0.75$, $q = 0.25$, $\alpha = 0.5$, $\beta = 0.6$, $\gamma = 0.1$ and $\delta = 0.2$. The full line shows the density $\langle \tau_{2x+1} \rangle$ and the dashed line the density $\langle \widehat{\tau}_{2x} \rangle$.

[3]) An implementation in C which takes care of all these details is available on the WWW under URL http://www.physik.fu-berlin.de/~ag-peschel/software/mp.html . This program does not only compute the current, the density profile and the two-point function on a finite chain, but also implements our results in Table 1 as well as the correlation length (4.6) and thus provides a simple way for checking their validity numerically.

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