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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.



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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 − 8]. They have also been encountered in diffusion-coagulation models [9]. 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 [10]. 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 $p = 1$, $q = 0$ [10]. 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 [11]. Alternating states were considered in [12, 13] 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 [14] 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 study of the two-dimensional representation provides an important clue to solving the problem in general. Namely, by using a certain relation between the operators, it is possible to eliminate the ones on one sublattice 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 [15] where the same algebra was used to describe the stationary state for a different dynamics where the updating is done step-by-step from one end of the chain to the other [1]). Using this connection, we can take over 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 leads to a mapping to the sequential case presented in Section 4. This is used in Section 5 to compute the current for general values of the parameters. Section 6 contains a discussion of the results and remarks on some other aspects as the relation to the model in [15] and the integrability of the model. A few computations are shifted to appendices which also 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 $\alpha$ and removed from it with probability $\gamma$. At the right boundary they are extracted with probability $\beta$ and added with probability $\delta$. 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 $T = T_2T_1$ 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 [15]. 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

$$
\begin{aligned}
T_1 &= \mathcal{L} \otimes \underbrace{\mathcal{T} \otimes \cdots \otimes \mathcal{T}}_{N/2-1 \text{ times}} \otimes \mathcal{R}\,, \\
T_2 &= \underbrace{\mathcal{T} \otimes \mathcal{T} \otimes \cdots \otimes \mathcal{T}}_{N/2 \text{ times}}\,,
\end{aligned}
\tag{2.1}
$$

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 [16, 17]. 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.

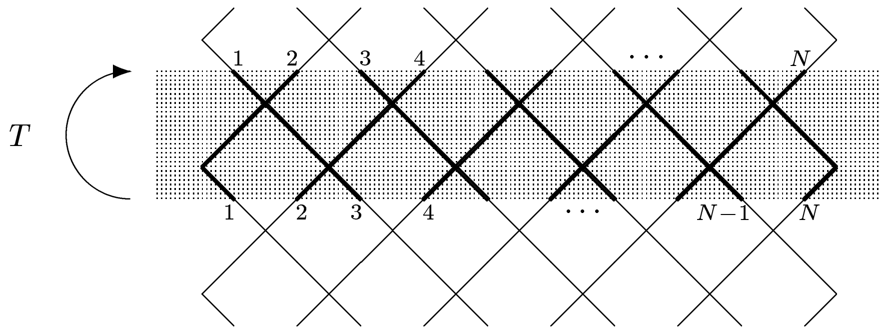



**Fig. 1:** Representation of the hopping processes as a vertex model. Only a part of the lattice is shown in the vertical direction. The shaded region contains all vertices that contribute to the diagonal-to-diagonal transfer matrix $T$.

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 [18]. 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.

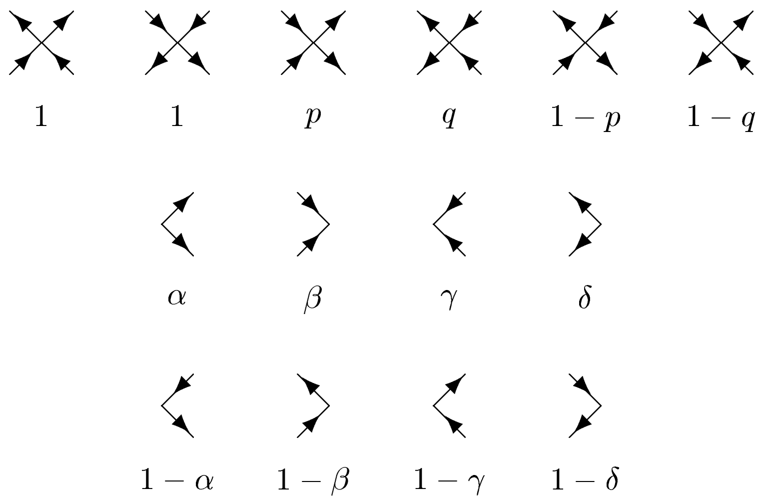



**Fig. 2:** The Boltzmann weights for the vertex model describing hopping with parallel dynamics.

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 [10] (and similarly [13]) 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

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

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

It has been argued in [10] 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 4.

The corresponding matrix-product state of the sequential limit is well-known (see e.g. [3, 19, 20]). 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 $\rho$. 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 $\rho$ 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 [21] with additional boundary terms $h_L$ and $h_R$ (see e.g. [20]). Since this Hamiltonian does not have any sublattice structure one can make a homogeneous 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, 19, 20] (see also [9]) 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, 19, 20]). The operator $C := E + D$ acts like a transfer matrix in the spatial direction and for example the density profile 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 motivations of this work 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. To explore this and the problem in general, we first study two special cases.

# 3. Direct solution

In this Section we solve (2.6) for the two simplest representations of the operators. This will indicate how to proceed in general.

First consider a *one-dimensional* representation, where the operators are represented by numbers, the boundary vectors can be discarded and one is dealing with a scalar product state. One finds that such a solution is possible if the relation

$$\begin{aligned} &(1-q)(\beta\gamma-\gamma-\beta+\beta\alpha)(\delta\alpha-\alpha-\delta+\beta\alpha) \\ &= (1-p)(\delta\gamma-\alpha-\delta+\delta\alpha)(\delta\gamma-\gamma-\beta+\beta\gamma) \end{aligned} \tag{3.1}$$

between the parameters holds. This condition is invariant under the simultaneous exchanges of $p$ with $q$, $\alpha$ with $\delta$ and $\beta$ with $\gamma$, which mirrors the reflection symmetry of the system. For $\gamma = \delta = 0$, (3.1) simplifies and becomes, for fixed $p$ and $q$, a hyperbola in the $\alpha-\beta$–plane which intersects the axes at $(p-q)/(1-q)$, see also [15]. In the sequential limit one recovers eq. (78) of [20].

More interesting is the case of a *two-dimensional* representation which is known to exist in the deterministic [10] and sequential limits [20]. Since, as mentioned above, the quantities

$$C := A + B\,, \qquad \widehat{C} := \widehat{A} + \widehat{B}\,, \tag{3.2}$$

will play the rôle of spatial transfer matrices, it is desirable that they have a particularly simple form. Summing the columns in (2.5) gives $[C, \widehat{C}] = 0$, so that they can be simultaneously brought into diagonal –or more generally Jordan normal– form. We will only consider the first case. It was shown in [10] that for invertible $C$, $\widehat{C}$ one can even choose

$$C = \widehat{C}\,. \tag{3.3}$$

A solution of the bulk equations (2.6a) with upper triangular $A$, $\widehat{A}$, $B$, $\widehat{B}$ and diagonal $C = \widehat{C}$ is

$$\begin{aligned} C &= \begin{pmatrix} 1 & 0 \\ 0 & -\frac{(\mathcal{A}(p-q)(p+q-1)+p(1-p))(\mathcal{A}(p-q)-p)}{(\mathcal{A}(p-q)-p+1)pq} \end{pmatrix}, \\ A &= \begin{pmatrix} -\frac{\mathcal{A}(q-1)}{\mathcal{A}(p-q)-p+1} & 1 \\ 0 & \frac{(q-1)(\mathcal{A}(p-q)-p)\mathcal{A}}{(\mathcal{A}(p-q)-p+1)p} \end{pmatrix}, \\ \widehat{A} &= \begin{pmatrix} \mathcal{A} & 1 \\ 0 & \frac{\mathcal{A}(\mathcal{A}(p-q)(p+q-1)+p(1-p))}{(\mathcal{A}(p-q)-p+1)p} \end{pmatrix}, \end{aligned} \tag{3.4}$$

with a free constant $\mathcal{A}$. Using (2.6b) and demanding non-trivial boundary vectors $|V\rangle$ and $|W\rangle$ then fixes it and also gives the following relation between the parameters:

$$f(p, q; \alpha, \beta, \gamma, \delta) = f(q, p; \delta, \gamma, \beta, \alpha) \tag{3.5a}$$

with

$$\begin{aligned} f(p, q; \alpha, \beta, \gamma, \delta) &:= (1-p)\,(1-q)\,p^3\alpha^2\beta^2 \\ &+ (1-p)\,pq^2\gamma\delta\left(\alpha\beta\,(1-q)^2 + (1-q)\,(q\,(\alpha+\beta) - (\delta\alpha+\beta\gamma)) - q\,((1-\gamma)\,\delta+\gamma-q)\right) \\ &+ p^2q^2\left(\alpha\,\gamma\,\left((1-\delta)^2-(1-\beta)^2\right) + q^2\gamma\,\delta\,(1-\alpha)\,(1-\beta)\right) \\ &+ p^2q^3\left(\beta\,\delta\,(1-\alpha)^2 + \alpha\,\gamma\,(1-\beta)^2 - \gamma\,\delta\,(1-\alpha)\,(1-\beta)\right)\,. \end{aligned} \tag{3.5b}$$

This is the condition for the existence of a two-dimensional matrix-product state.

Obviously, (3.5) is rather complicated in general. As before, choosing $\gamma = \delta = 0$ leads to a marked simplification. Then one has, for $p \neq 0$, $\alpha \neq 0 \neq \beta$

$$(1-q)\{(1-p-q)\alpha\beta + q(\alpha+\beta)\} = q(p-q)\,. \tag{3.6}$$

which is another hyperbola in the $\alpha$-$\beta$–plane, but with the same intersection points as for the scalar case.

In the sequential limit, eq. (81) of [20] is re-obtained from (3.5). Finally, for deterministic hopping to the right, i.e. $p = 1$ and $q = 0$, the condition (3.5) is satisfied automatically. This is consistent with [10] where a two-dimensional representation for $\gamma = \delta = 0$ was found. However, one cannot set $p = 1$ in our solution, because then singularities appear in (3.4).

One may wonder if the conditions (3.1), (3.5) for the two types of product states are linked to the specific mechanism (2.4) and (2.5). However, one can eliminate the alternating structure by working with block-spin variables for two neighbouring sites. Then one can show, using just short chains, but no specific mechanism, that a homogeneous matrix-product ansatz with $N$-independent matrices leads again to (3.1), and at least for $\gamma = \delta = 0$, also (3.6) is obtained.

With these explicit solutions it is straightforward to calculate physical quantities like the density profile, the current or the correlation length. Using proper variables, the results can be written in compact form. This is sketched in appendix A.

More important here is the following observation: The matrices in (3.4) satisfy

$$A - \widehat{A} = \widehat{B} - B = \frac{\mathcal{A}(1-\mathcal{A})(p-q)}{1-p+(p-q)\mathcal{A}}\mathbb{1} =: g(p, q; \alpha, \beta, \gamma, \delta)\mathbf{1}, \tag{3.7}$$

i.e. the differences are multiples of the unit matrix. An analogous results holds trivially in the one-dimensional case. Using now (3.7) to eliminate $\widehat{A}$ and $\widehat{B}$, the conditions (2.6) turn into

$$\begin{aligned} \langle W|\,(\alpha A - \gamma B) &= g\,\langle W|\,, \\ (\beta B - \delta A)\,|V\rangle &= g\,\,(1-\beta-\delta)\,|V\rangle\,, \\ pBA - qAB &= g\,\,(((1-q)B + (1-p)A)\,. \end{aligned} \tag{3.8}$$

This looks very similar to the relations (2.12) of the sequential limit and can be used in two ways.

Firstly, one can indeed recover (2.12) by using (2.7) and taking $\rho$ to zero. Then all operators as well as the boundary vectors have finite limits, the sublattice structure vanishes and the function $g$ in (3.7) behaves as $g(p,q;\alpha,\beta,\gamma,\delta) \approx \rho\,\widehat{g}(\widehat{p},\widehat{q};\widehat{\alpha},\widehat{\beta},\widehat{\gamma},\widehat{\delta})$. Dividing by $\widehat{g}$ and setting finally $E := A/\widehat{g}$, $D := B/\widehat{g}$, one recovers precisely (2.12). This shows how one mechanism goes over into the other.

Secondly, one can relate (3.8) to (2.12) quite generally. This provides a way to treat the parallel dynamics problem for arbitrary representations with the property (3.7) and is done in the following.

# 4. Mapping onto the Hamiltonian limit

In this Section we map the problem for parallel dynamics to the one with sequential dynamics. We impose the condition (3.7) with $g = 1$ (which corresponds to a different normalization of $A$, $B$, $\widehat{A}$ and $\widehat{B}$) for general values of the parameters, so that

$$\widehat{B} - B = A - \widehat{A} = \mathbb{1} \tag{4.1}$$

holds (This has also been proposed in [15]). 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 (4.1) holds. We will now show that (4.1) 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 $\alpha$, $\beta$, $\gamma$, $\delta$, $p$ 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 (4.1) is valid. Thus, from a physical point of view it is completely sufficient to study only representations satisfying (4.1).

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 $D$:

$$\begin{aligned} A &= n_E E + e\mathbb{1}\,, \qquad & \widehat{A} &= n_E E - (1-e)\mathbb{1}\,, \\ B &= n_D D - d\mathbb{1}\,, \qquad & \widehat{B} &= n_D D + (1-d)\mathbb{1}\,, \end{aligned} \tag{4.2}$$

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 $D$:

$$\begin{aligned} n_E n_D (pDE - qED) =& n_E E \left(d(p-q) + (1-p)\right) + n_D D \left(-e(p-q) + (1-q)\right) \\ &+ ed(p-q) + e(1-p) - d(1-q)\,. \end{aligned} \tag{4.3}$$

In order to be able to identify this with (2.12) the constant term in (4.3) must vanish. This is ensured by choosing

$$e = \frac{d(1-q)}{d(p-q) + (1-p)}\,. \tag{4.4}$$

Also the linear term in $E$ must appear with the same coefficient as the linear term in $D$ on the r.h.s. of (4.3). This is the case if

$$n_D = -n_E \frac{d(p-q)+(1-p)}{e(p-q)-(1-q)} = n_E \frac{(d(p-q)+(1-p))^2}{(1-p)(1-q)} \,. \tag{4.5}$$

Using (4.4) and (4.5) the relation (4.3) now reads

$$n_E \frac{d(p-q)+(1-p)}{(1-p)(1-q)} (pDE - qED) = E + D \,. \tag{4.6}$$

Inserting the ansatz (4.2) into the boundary equations (2.6b) leads to

$$\langle W| \frac{\alpha n_E E - \gamma n_D D}{1-\alpha e - \gamma d} = \langle W| \,, \qquad \frac{\beta n_D D - \delta n_E E}{1+\delta e+\beta d-(\delta+\beta)} |V\rangle = |V\rangle \,. \tag{4.7}$$

The equations (4.6) and (4.7) are identical to the algebra of the sequential limit (2.12) if one identifies the rates in that limit as follows

$$\begin{aligned}
\widehat{p} &= n_E \frac{d(p-q)+(1-p)}{(1-p)(1-q)} p \,, & \widehat{q} &= n_E \frac{d(p-q)+(1-p)}{(1-p)(1-q)} q \,, \\
\widehat{\alpha} &= n_E \frac{1}{1-\alpha e-\gamma d} \alpha \,, & \widehat{\beta} &= n_D \frac{1}{1+\delta e+\beta d-(\delta+\beta)} \beta \,, \\
\widehat{\gamma} &= n_D \frac{1}{1-\alpha e-\gamma d} \gamma \,, & \widehat{\delta} &= n_E \frac{1}{1+\delta e+\beta d-(\delta+\beta)} \delta \,.
\end{aligned} \tag{4.8}$$

Here, the constants $e$ and $n_D$ are fixed by (4.4) and (4.5). 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 $\widehat{q} = q$. Also any other choice for $n_E$ is permitted because $n_E$ has to disappear from the final result for any physical quantity. In the following we choose $n_E = 1$ in order to simplify the presentation, but we have also checked that if it is kept, the final results are manifestly independent of it. Also the constant $d$ is still free in (4.8) and for explicit computations it will be fixed to a value that ensures $n_D = n_E$ $(= 1)$. This choice is crucial, because then $A+B = E+D+(e-d)$ and the operators $C$ for the parallel and sequential case may be identified with each other.

From (4.8) 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 (4.5). 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 (4.8) where $n_E$ and $d$ are kept as free parameters into the conditions for the sequential limit [20]. The $d$-independent factors of these renormalized conditions are precisely (3.1) and (3.5) 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 [20]. However, the operators $C$ in the two cases differ by the additive constant $e-d$ and therefore results for expectation values in the parallel case cannot be simply taken from the sequential limit.

# 5. Current and phase diagram

Now we show how to use the mapping of the previous Section to compute the current, following the treatment in [19] of the sequential case.

According to [19, 20], the phase diagram in the sequential case is given by a single function $\kappa_+$ 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 the parallel case, if the quantities (4.8) are inserted into the functions $\kappa_+$. To be more precise, the parallel case will be described 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 [19, 20] by choosing the constant $d$ in the mapping (4.8) such that $n_D=n_E$ $(=1)$. Explicitly one finds

$$\begin{aligned}\widehat{\kappa}_\pm(x,y)=&\frac{1}{2x\sqrt{(1-q)\,(1-p)}}\Big(-x(1-q)+y(1-p)+p-q\\&\pm\sqrt{(-x(1-q)+y(1-p)+p-q)^2+4xy\,(1-q)\,(1-p)}\Big)\,.\end{aligned}\tag{5.1}$$

The quantities $\widehat{\kappa}_+$ may be regarded as effective input/output rates at the boundaries and should be used only for $p>q$ (results for the case $p<q$ can be obtained by applying parity, i.e. by exchanging $p$ with $q$, $\alpha$ with $\delta$ and $\beta$ with $\gamma$). For a more detailed discussion compare appendix A.

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

$$\widehat{J}=p\widehat{B}A-q\widehat{A}B\,.\tag{5.2}$$

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. Using (2.6b) and the ansatz (4.1) one can check that in all three cases

$$J=\frac{\langle W|C^{N-1}|V\rangle}{\langle W|C^N|V\rangle}\tag{5.3}$$

holds. 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 (4.1) 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 (4.2) that

$$C=A+B=E+D+(e-d)\,.\tag{5.4}$$

In [19] 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

$$D=\frac{F+1}{\widehat{p}-\widehat{q}}\,,\qquad E=\frac{F^\dagger+1}{\widehat{p}-\widehat{q}}\,.\tag{5.5}$$

Inserting this into (5.4) leads to

$$C = \frac{F + F^\dagger + \lambda}{\widehat{p} - \widehat{q}} \tag{5.6}$$

with

$$\lambda = 2 + (e-d)(\widehat{p} - \widehat{q}) = \frac{2-q-p}{\sqrt{(1-q)(1-p)}} \,. \tag{5.7}$$

First we consider the case $\widehat{\kappa}_+(\alpha,\gamma) < 1$ and $\widehat{\kappa}_+(\beta,\delta) < 1$ which corresponds to phase III below. According to [19] 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 $\lambda$ because of the extra constant in (5.6). Tracing the effect of this modification one finds that for parallel dynamics the current in the maximal current phase is given by

$$J = \frac{\widehat{p} - \widehat{q}}{2+\lambda} = \frac{\sqrt{1-q} - \sqrt{1-p}}{\sqrt{1-q} + \sqrt{1-p}} \,. \tag{5.8}$$

The currents for the other two phases can be obtained from similar modifications of the computations in [19]. It is sufficient to perform this computation for $\widehat{\kappa}_+(\beta,\delta) > \widehat{\kappa}_+(\alpha,\gamma)$ and $\widehat{\kappa}_+(\beta,\delta) > 1$ which will correspond to phase I. The relation (4.7) of [19] remains valid with the new parameters and reads

$$\langle W|C^{N-1}F|V\rangle \approx \kappa_+(\widehat{\beta},\widehat{\delta})\langle W|C^{N-1}|V\rangle = \widehat{\kappa}_+(\beta,\delta)\langle W|C^{N-1}|V\rangle \,. \tag{5.9}$$

One can further rewrite $C$ as follows using (5.4) – (5.7)

$$\begin{aligned} C =& \frac{1}{\widehat{\delta}}\left( -(\widehat{\beta}D - \widehat{\delta}E) + \frac{\widehat{\beta} + \widehat{\delta} + \widehat{\delta}\,(\widehat{p} - \widehat{q})(e-d)}{\widehat{p} - \widehat{q}} + \frac{\widehat{\beta} + \widehat{\delta}}{\widehat{p} - \widehat{q}}F \right) \\ =& \frac{1}{\widehat{\delta}}\left( -(\widehat{\beta}D - \widehat{\delta}E) + \frac{\widehat{\beta} + \widehat{\delta} + \widehat{\delta}(\lambda - 2)}{\widehat{p} - \widehat{q}} + \frac{\widehat{\beta} + \widehat{\delta}}{\widehat{p} - \widehat{q}}F \right) \,. \end{aligned} \tag{5.10}$$

Making first use of (5.10) and then of (5.9) one finds the following recurrence relation for the normalization constants (generalizing eqs. (4.8) and (4.9) of [19])

$$\begin{aligned} &\langle W|C^N|V\rangle \\ &= \frac{1}{\widehat{\delta}}\,\frac{1}{\widehat{p} - \widehat{q}}\left\{ \left(\widehat{\beta} + \widehat{\delta} + \widehat{\delta}(\lambda-2) - \widehat{p} + \widehat{q}\right)\langle W|C^{N-1}|V\rangle + \left(\widehat{\beta} + \widehat{\delta}\right)\langle W|C^{N-1}F|V\rangle \right\} \\ &\approx \frac{1}{\widehat{\delta}}\,\frac{1}{\widehat{p} - \widehat{q}}\left\{ \left(\widehat{\beta} + \widehat{\delta} + \widehat{\delta}(\lambda-2) - \widehat{p} + \widehat{q}\right) + \left(\widehat{\beta} + \widehat{\delta}\right)\widehat{\kappa}_+(\beta,\delta) \right\}\langle W|C^{N-1}|V\rangle \,. \end{aligned} \tag{5.11}$$

Inserting this result into (5.3) one arrives after a straightforward computation at the formula presented in Table 1. The result for the other case $\widehat{\kappa}_+(\alpha,\gamma) > \widehat{\kappa}_+(\beta,\delta)$ and $\widehat{\kappa}_+(\alpha,\gamma) > 1$ (phase II) can be obtained simply by replacing $\beta$ by $\alpha$ and $\delta$ by $\gamma$.

These results can be verified using the one- and two-dimensional representations of Section 3 (compare appendix A). In the limit of small probabilities the formulae for the current in all three phases go into the ones obtained for sequential dynamics, namely eqs. (4.6), (4.10) and (4.11) of [19], respectively.

| *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:** Results for the current $J$ and the bulk densities $\langle \tau_x \rangle$, $\langle \widehat{\tau}_x \rangle$ on the odd and even sublattices, respectively. Formulae containing $\widetilde{\kappa}_\pm = \sqrt{(1-q)\,(1-p)}\,\widehat{\kappa}_\pm$ are valid for $p > q$.

Table 1 also contains results for the densities at the even and odd sites in the bulk of the system, where in regions I and II it is approximately constant. These were obtained for the lines (3.1), (3.5) using the explicit one- and two-dimensional representations of Section 3, as outlined in appendix A. They can be used to classify the regions I and II according to high and low densities, respectively. The formulae are also written in terms of $\widetilde{\kappa}_+$, since for example numerical computations (as described in appendix B) indicate that they hold in the entire regions I and II. On the coexistence line $\widehat{\kappa}_+(\alpha,\gamma) = \widehat{\kappa}_+(\beta,\delta)$ which separates these two regions the density profile is linear in space. This corresponds to representations where $C$ has a non-trivial Jordan form.

In addition, one can also obtain an expression for the correlation length (see appendix A) that, according to the numerical computations outlined in appendix B, seems to be valid in the parts of phases I and II where $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) > 1$,

All 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 [19, 20]. 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:

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)

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. All our results have the correct behaviour under this duality transformation.

The dotted line in Fig. 3 shows the condition (3.1) 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 (3.5) 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 (3.5). 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.

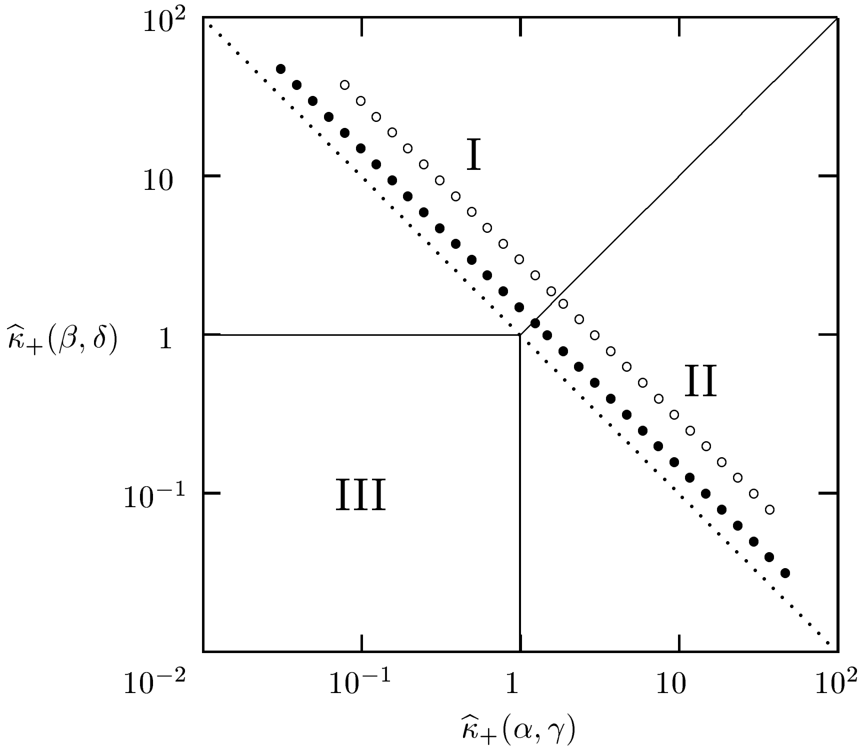



**Fig. 3:** Phase diagram of the kinetic model. The dotted line shows the condition (3.1) for a one-dimensional representation. The condition (3.5) for a two-dimensional representation is shown for two choices of $p$ and $q$: The symbol '$\circ$' is for $p = 0.75$, $q = 0.25$ and the symbol '$\bullet$' is for $p = 0.6$, $q = 0.4$.

For a more detailed discussion of the case $\gamma = \delta = 0$ we refer to [22].

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 explain how to use (3.7) with $g = 1$ for numerical computations on finite chains. In this manner one can e.g. check the results of this Section and appendix A. In appendix C we show how one can use the same representation to compute correlation functions for the case of symmetric diffusion $p = q$ where the results of this Section and appendix A may not be applied directly, but where the algebra is much simpler.

## 6. 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.

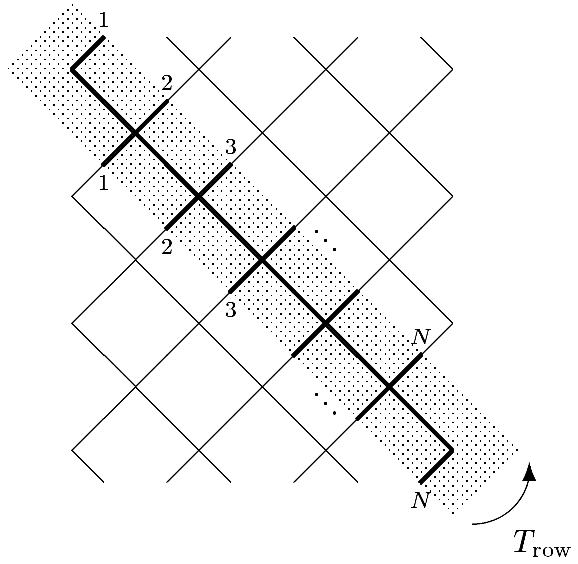
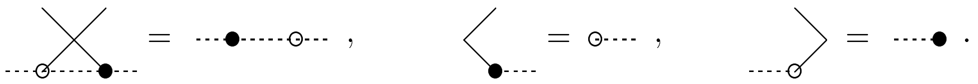



**Fig. 4:** Representation of a step-by-step dynamics starting at the right end of the system as a vertex model.

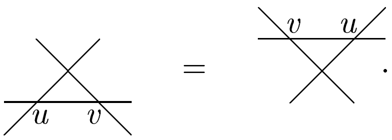
In [15] it was found that the same is true for yet another type of dynamics, where the stochastic motion takes place step-by-step along the chain. This can be visualized nicely in the vertex-model picture as shown in Fig. 4. The processes take place in a diagonal strip of the lattice and the time-evolution operator is seen to be the usual row-to-row transfer matrix $T_{\text{row}}$ 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 homogeneous 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) [15].

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 [13]):



(6.1)

The first identity is strikingly similar to the Yang-Baxter equation (see e.g. Chapter 2.3 of [23]) which for vertex models reads graphically




(6.2)

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 [24, 25]. One would expect that this also holds for the full vertex model. A proof would have to follow the lines of [24 – 26]. 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 [11] show that this cannot be true in general. Nor does the construction in [27] ensure integrability. It amounts to transforming the bulk relation in (6.1) into a commutator as in (6.2) 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 [28] and the stationary state has been shown to have a matrix-product form with four-dimensional matrices [9]. As in the present work, there are four matrices involved, two for the homogeneous 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 identity and thus one would find the more general matrix-product mechanism of [9] 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 [9] 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 [29]. For a certain fixed particle density, the stationary state is also expressible in the form of a two-dimensional matrix product [30]. One may speculate that our representation (3.4) 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 4 and 5 may be useful also for systems with a defect.

## Acknowledgments

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## Appendix A. Physical quantities

Given the explicit representations of Section 3, one can determine e.g. current, density or correlation length in the stationary state. This provides a physical picture and also a check on the results for the current obtained in a different way in Section 5.

The current is particularly simple because it is independent of position. For the scalar product state one finds, using the expression $J = (\alpha A - \gamma B)/C$ at the left boundary:

$$J = \frac{\alpha\beta - \gamma\delta}{\alpha + \beta + \gamma + \delta - (\alpha + \gamma)(\beta + \delta)} \,. \tag{A.1}$$

However, this is valid under the constraint (3.1) and can therefore be brought into various other forms. It turns out that the appropriate variable is the $\widetilde{\kappa}_+$ introduced in Section 5. Then $J$ can be written in the two forms given in Table 1. For the two-dimensional representation (3.4) the current depends on the length $N$, but the limit $N \to \infty$ can still be computed easily upon observing that only matrix elements corresponding to the largest eigenvalue of $C$ contribute to this limit. For the two-dimensional matrix-product state this leads to the distinction between region I defined by $C_{2,2} > C_{1,1}$ and region II in the other case. One finds that the expressions in Table 1 also hold for the two-dimensional matrix-product state.

The same feature is found for the density which is given by $\langle \tau_x \rangle = \langle W | C^{x-1} B C^{N-x} | V \rangle / \langle W | C^N | V \rangle$ for $x$ odd and by an analogous expression $\langle \widehat{\tau}_x \rangle$ with $B \to \widehat{B}$ for $x$ even. These quantities are independent of $x$ for the scalar product state. This is not the case for the two-dimensional representation (3.4), but in the bulk the densities become constant and can be computed again from appropriate matrix elements, e.g. $\langle \tau_x \rangle = B_{1,1}/C_{1,1}$ for region II. Expressing them in terms of $\widetilde{\kappa}_+$ one obtains for both product states the forms given also in Table 1. Note that in the sequential limit $\langle \widehat{\tau}_x \rangle \to \langle \tau_x \rangle$ and we recover the result eq. (100) of [20]. For the special case $\gamma = \delta = 0$ the expressions for the densities simplify to

$$\langle \tau_x \rangle = 1 - \beta \frac{1-q}{p-q} \,, \qquad \langle \widehat{\tau}_x \rangle = \frac{1}{1-\beta} \langle \tau_x \rangle \,, \tag{A.2a}$$

$$\langle \tau_x \rangle = \frac{\alpha}{1-\alpha} \frac{1-p}{p-q} \,, \qquad \langle \widehat{\tau}_x \rangle = (1-\alpha) \langle \tau_x \rangle + \alpha \,, \tag{A.2b}$$

for region I or II, respectively.

Finally, the correlation length $|\zeta|$ for the two-dimensional product state is given by $\exp(1/\zeta) = C_{2,2}/C_{1,1}$ and can again be written in terms of $\widetilde{\kappa}_+$:

$$\exp\left(\frac{1}{\zeta}\right) = \frac{\widetilde{\kappa}_+(\alpha,\gamma)\,(1 - p + \widetilde{\kappa}_+(\beta,\delta))\,(1 - q + \widetilde{\kappa}_+(\beta,\delta))}{\widetilde{\kappa}_+(\beta,\delta)\,(1 - p + \widetilde{\kappa}_+(\alpha,\gamma))\,(1 - q + \widetilde{\kappa}_+(\alpha,\gamma))} \,. \tag{A.3}$$

To be precise, we have established (A.3) analytically for either $\gamma = 0$ or $\delta = 0$. For both probabilities non-zero we have performed a careful numerical verification. As expected, the result eq. (102) of [20] is recovered in the sequential limit.

The result (A.3) can also be used to translate the inequalities between $C_{2,2}$ and $C_{1,1}$ into such between $\widehat{\kappa}_+(\alpha,\gamma)$ and $\widehat{\kappa}_+(\beta,\delta)$. On the manifold (3.5) one finds numerically that $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) > 1$. This can be used to infer from (A.3) that $C_{2,2} > C_{1,1}$ iff $\widehat{\kappa}_+(\beta,\delta) > \widehat{\kappa}_+(\alpha,\gamma)$ so that phase I is characterized by either condition.

The results cited so far are not confined to the manifolds for which they were derived. In the case of the current, the treatment of Section 5 shows that the formulae are valid in the whole regions I and II. For the densities this has not been proven but there is strong numerical evidence for it, compare also [20]. Similarly, it is likely that (A.3) holds for all parameter values with $\widehat{\kappa}_+(\alpha,\gamma)\widehat{\kappa}_+(\beta,\delta) > 1$. The boundary of this region is determined by the scalar product state, and the correlation length diverges as one approaches it.

Finally, let us comment on the $\widetilde{\kappa}_\pm$ which plays the rôle of a uniformization variable. Consider first the case $\gamma = \delta = 0$. Then $\widetilde{\kappa}_+(x,0) = -(1-q) + (p-q)/x$ and $\widetilde{\kappa}_-(x,0) = 0$, i.e. for $p \neq q$ the quantity $\widetilde{\kappa}_+(x,0)$ is basically the inverse of the probability $x$ which is related to particle input (if $x = \alpha$) or output (if $x = \beta$). For $y > 0$, the quantity $\widetilde{\kappa}_+(x,y)$ can be thought of as an effective input and output rate. For example, for small hopping probabilities in the bulk ($p, q \to 0$) one has $\widetilde{\kappa}_+(x,y) \approx y/x$. In general, $\widetilde{\kappa}_+$ takes into account the effect that a particle is injected, travels into the system, returns and is removed at the same boundary.

# Appendix B. Computations on finite chains

We show here how to compute correlation functions efficiently using a representation of the algebra where (4.1) holds. Then $A$ and $B$ satisfy (3.8) 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

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

The bulk relation in (3.8) (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

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

for $y > 0$. As soon as the operator $A$ hits the right boundary one can use the second boundary equation in (3.8) with $g = 1$ to replace $A$ by $B$:

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

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

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

The rules (B.2) – (B.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 (3.8) (with $g = 1$). This leads to

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

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 (B.2) – (B.5).

It is possible to solve these recurrence relations in closed form following the lines of [19]. However, also formulae of the type as in [19] 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 [2]).

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 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 (5.3): $J = 0.2690$. This is to be compared to the result $J = 0.2679$ obtained from (5.8) in the thermodynamic limit. Computations like this one provide room for more detailed investigations.

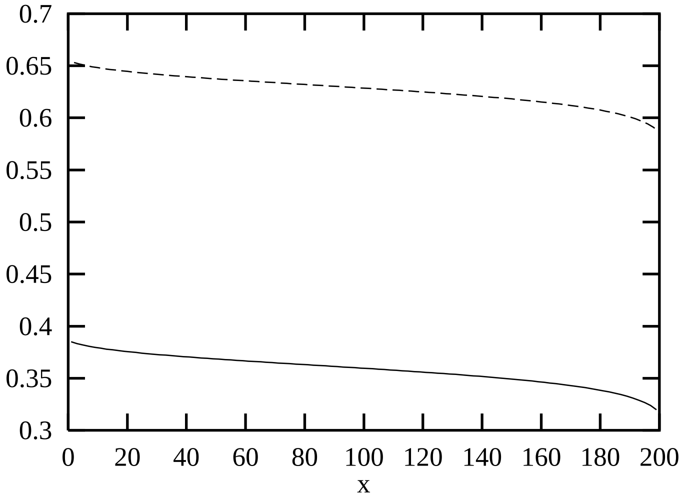


**Fig. 5:** A density profile in the maximal current phase with $N = 200$ sites and $p = 0.75$, $q = 0.25$, $\alpha = 0.5$, $\beta = 0.6$, $\gamma = 0.1$ and $\delta = 0.2$. The full line shows the density $\langle\tau_{2x+1}\rangle$ and the dashed line the density $\langle\widehat{\tau}_{2x}\rangle$.

[2]) 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 (A.3) and thus provides a simple way for checking their validity numerically.

## Appendix C. 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 [16], it is convenient to work with the operator $B$ and the spatial transfer-matrix $C$. Inserting the choice (4.1) into (2.6) leads to

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

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

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

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

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

A similar computation with $\widehat{B} = B + \mathbb{1}$ yields the profile for the even sites. The expression differs from (C.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 [31] for the case of sequential updates.

For finite $N$, the density profile (C.3) is linear in the spatial variable $x$ (as one can already see from (C.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 (C.3) one finds that

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

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 (C.3) and (C.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.

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