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Shocks in the asymmetric simple exclusion process in a discrete-time update

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Abstract. We study the dynamics of a shock distribution as an initial state for a one-dimensional asymmetric simple exclusion process with sub-lattice parallel update. The time evolution of the shock distribution can be calculated exactly if the two initial densities of the shock satisfy a special relation which results from its $U_q[SU(2)]$ symmetry. The resulting distribution is a linear combination of shock measures. The motion of the shock position can be interpreted as if it would perform a biased discrete-time random walk, with hopping rules related to that of a single particle in the exclusion process. The shock diffusion constant and the shock velocity are calculated exactly. We obtain simple expressions for these quantities in terms of the shock densities and currents which we argue to be valid for any pair of shock densities.

1. Introduction

The exploration of exclusion processes plays an important part in special fields of many-body systems, for example the study of traffic (jams) [1], tagged-particle diffusion (e.g. in zeolites) [2], reading processes for RNA strands within cells [3] or the description of motion of entangled polymers [4].

The asymmetric simple exclusion process (ASEP) is a model of diffusing identical particles with hard-core interaction on a lattice. Every single particle performs a biased random walk, but at the same time they obey the exclusion principle which prohibits the occupation of a lattice site by more than one particle. A considerable amount of exact results including stationary states, correlation functions and lengths were obtained by using probabilistic tools [5], the Bethe ansatz and related quantum mechanical methods [6] or the matrix product ansatz [7].

In this paper we will concentrate on the temporal evolution of a shock in a special ASEP. We calculate the full time evolution of an initial shock measure which will be shown to evolve into a linear combination of similar shock distributions if a particular constraint between hopping probabilities of the exclusion particles and the shock densities is fulfilled. It will transpire that the shock—which represents the collective motion of many particles—may be described by only one parameter, the shock position. This position represents the increase or decrease of the densities in the ensemble average. Such a reduced description in terms of the stochastic dynamics of a single coordinate can be motivated by the every day experience of traffic jams, but also by Monte Carlo simulations of the exclusion process [8, 9] where the existence of a sharp shock is not *a priori* clear. We stress that the particle dynamics in the exclusion process takes place on a microscopic scale whereas quantities like the shock positions usually appear

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in a macroscopic framework of some description†. It is well known that on a macroscopic level corresponding to the Euler scale a shock can be viewed as a collective single particle excitation. However, usually the macroscopic results are only approximate but not exact due to the reduction of the degrees of freedom. Hence it is surprising that this exclusion model yields *exact* single-particle dynamics for the shock even on the microscopic lattice scale. Thus we are furnished with a nice, but rare instance where the emergence of macroscopic degrees of freedom can be directly deduced from microscopic scales without invoking any approximation or taking any scaling limit.

A few remarks on related work are relevant here. There are studies of the time evolution of shocks for the continuous-time exclusion process which involve the introduction of so-called second-class particles [10, 11]. This technique yields exact (and rigorous) results in certain scaling limits without constraints on the hopping rates and boundary densities of the shock. In our approach second-class particles do not appear. Instead we make use of a quantum algebra symmetry of the generator of the process (first pointed out in [12,13]) which allows us to directly relate the time evolution of a shock to the time evolution of a single particle if the boundary densities of the inital shock measure satisfy a specific relation involving the right/left hopping rates. This approach was employed in recent work on the continuous-time ASEP [14] to obtain rigorously the time evolution of shock measures. Here we discuss a discrete-time exclusion process with sub-lattice update and a corresponding sub-lattice structure of the stationary distribution. This generalized model includes the continuous-time process as the limiting case where all hopping probabilities tend to zero (see section 3 where a precise definition of the model is given). Our results differ from those of [14] in various aspects related to the sub-lattice nature of the dynamics and—more importantly—in the exact expression for the diffusion coefficient of the shock derived below.

From a mathematical angle it is also interesting to note that while the quantum algebra symmetry requires us to take the thermodynamic limit, a single-shock picture remains valid also in the continuous-time exclusion process on a finite lattice with open boundaries if a constraint on the boundary injection/absorption rates analogous to our constraint is satisfied [15]. It would be interesting to investigate whether this extends to the ASEP studied here, but also on a finite lattice with open boundaries. This is, however, not the objective of this paper which deals only with the thermodynamic limit.

Finally, we point out that unlike in the studies using second-class particles we work on the lattice scale without taking scaling limits. However, we restrict ourselves to a one-parameter family of shock measures which satisfy the constraint referred to above. Even though we repeatedly refer to the quantum algebra symmetry of the process which leads to this constraint, this symmetry does not enter explicitly in our calculations. We only make use of one consequence—the closure of the equations of motion for a certain family of observables; see section 3.3—which is crucial to the derivation of the time evolution of the shock measure. For more details we refer to [16] where the closure of the equations of motion is derived and discussed in some detail.

The paper is organized as follows. In section 2 we set up the formalism in which we shall present the exclusion process (section 3) and which allows us to use the quantum mechanical tools required for reducing the shock dynamics to single-particle dynamics. This is also the subject of section 3 where the main result, the time evolution of an initial shock measure, is presented. Expressing the exact drift velocity and diffusion constant of the shock in terms of

† More precisely speaking a lattice gas description refers to a mesoscopic scale rather than a microscopic one, governed by Newtons or quantum mechanical equations of motion. However, it has become customary to use the notion microscopic for lattice gas models, particularly when this is meant in contrast to the macroscopic hydrodynamical approach.

the currents and densities characterizing the initial shock distribution allows us to draw some conclusions which may be valid in more general settings (section 4). In the appendix we analyse the properties of the associated single-particle random walk.

2. The quantum Hamiltonian formalism

We want to apply the 'quantum Hamiltonian' formalism [6], which was originally introduced for spin systems [17] and later also for 'bosonic' systems where particles do not have excluded volume [18–21], and for exclusion models [22, 23]. The starting point is a balance equation, the master equation, which connects the probabilities $P(n, t)$ of states n at time t. Formally, it can be written in the following discrete manner:

$$P(n, t + \Delta t) = \sum_m p_m^n P(m, t). \tag{1}$$

The system evolves from a set of states m with the transition probabilities $p_m^n \in [0, 1]$ to the unique state n during one time step Δt. Later, m and n will represent lattice vectors over all occupation numbers $\in 0, 1$.

To set up the quantum Hamiltonian formalism let us introduce a vector space (Fock space) where each state n is assigned to a vector $|n\rangle$ (or to $\langle n|$, its dual vector) with scalar product $\langle n|m\rangle = \delta_{m,n}$. These states represent possible particle configurations at different lattice sites. Then the total temporal evolution of the probability vector $|P(t)\rangle$ starting with the initial state $P(t)$ during Δt can be expressed by

$$|P(t + \Delta t)\rangle = T|P(t)\rangle \tag{2}$$

since T is the stochastic transfer matrix. Its formal solution is given by

$$|P(t)\rangle = |P(n\Delta t)\rangle = T^n|P(0)\rangle \tag{3}$$

if $|P(0)\rangle$ is the initial distribution and $t = n\Delta t$. The probability vector can be decomposed into the state vectors $|n\rangle$ by using the probabilities $P(n, t)$

$$|P(t)\rangle = \sum_n P(n, t)|n\rangle. \tag{4}$$

For a lattice system of size $4L$ with site occupation numbers $n_k \in \{0, 1\}$ the state $|n\rangle = \bigotimes_{k=-2L+1}^{2L} |n_k\rangle$ is the tensor product of all local states over the lattice. We choose a basis such that $|n_k = 1\rangle = (\,0 \quad 1\,)^T$ if the position k is occupied by a particle and $|n_k = 0\rangle = (\,1 \quad 0\,)^T$ otherwise. The expectation value of an arbitrary quantity G is given by

$$\langle G\rangle = \sum_{\vec{n}} G(\vec{n})P(\vec{n}, t) \tag{5}$$

and represents the expectation values over many realizations of the same process (ensemble average). In the Fock space this can be expressed by

$$\langle G\rangle = \langle \vec{r}|G|P(t)\rangle \tag{6}$$

where $\langle \vec{r}| = \langle r|^{\otimes 4L}$ and $\langle r| = (\,1 \quad 1\,)^T$ is the reference vector which has all components equal to 1. This implies that G has a diagonal form $G = \sum_n G(n)|n\rangle P(n, t)\langle n|$. As a special case

$$\rho_i = \langle \vec{r}|n_i|P(t)\rangle \tag{7}$$

we find the expectation value for the density if n_i is the number operator of the lattice site i. The evolution of G is performed by the action of the transfer matrix T on the probability vector

$$\langle G(t)\rangle = \langle \vec{r}|GT^n|P(0)\rangle. \tag{8}$$

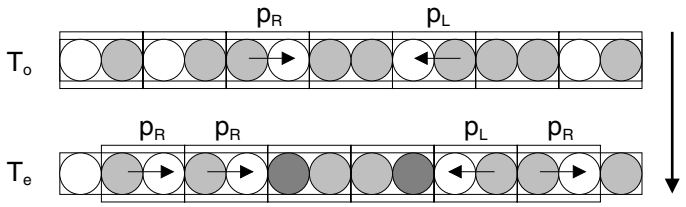

Figure 1. Parallel update sequence of a ASEP (in direction of the large arrow on the rhs). Small arrows indicate possible jumps. Each cell represents a lattice site. Particles which have moved in the first half step (odd sub-lattice) are shown in dark grey in the second half step.

The conservation of the total probability

$$1 = \sum_n P(n,t) = \langle \vec{r}|P(t)\rangle \forall t \tag{9}$$

implies that $\langle \vec{r}|$ is an eigenvector of T

$$\langle \vec{r}|T = \langle \vec{r}| \tag{10}$$

with eigenvalue 1. That means simply that the sum of all transition probabilities is equal to 1.

A probability distribution $|P(t)\rangle$ which is invariant under time translation T is called stationary. We denote it by $|P^*\rangle$. The diagonal matrix which has the stationary probabilities as the diagonal elements is denoted by P^*. Hence we have

$$T|P^*\rangle \equiv T P^*|\vec{r}\rangle = |P^*\rangle. \tag{11}$$

The stationary state $|P^*\rangle$ is usually not identical to $|\vec{r}\rangle$ but is a more complex object.

3. Shock motion in the sub-lattice ASEP

3.1. The asymmetric exclusion model

Following the idea proposed in [24,25] we study an exclusion process which can be connected to a six vertex model [26]. In a chain of length $4L$ (beginning from $-2L+1$) every lattice site can be occupied by a particle or not. The constraint of a finite chain will be lifted later for an infinite chain in the thermodynamic limit. We include hard-core interaction between the particles, so if one place is occupied by a particle no other one can jump on it. The stochastic time evolution of the system proceeds in two half-time steps. For this purpose we will divide the chain into pairs of sites as shown in figure 1.

(1) We choose the pairs for the first half-time step, $t \to t + \frac{1}{2}$, in such a way that the first lattice index is odd. That is, $(-2L+1, -2L+2) \ldots (2L-1, 2L)$ form pairs, and the evolution only takes place between these two lattice points in a parallel update. Hence, if both sites are occupied or empty, they remain unchanged. However, if one of these sites is empty and the other not, the particle jumps onto it with probability p_L (p_R) if the jump is to the left (right).

(2) In the second half-time step, $t+\frac{1}{2} \to t+1$, the pairing is shifted by one lattice unit and the even pairs $(-2L+2, -2L+3) \ldots (2L-2, 2L-1)$ will be updated in the same manner as above. Notice that the first and the last site are excluded in this update step whereas the boundary sites are involved during the first time step.

With this choice of reflecting boundary conditions the model satisfies detailed balance. The steady state is identical to that of the usual exclusion process in continuous-time and

is described in detail in [13]. The continuous-time exclusion process is obtained from the discrete-time model by taking the limit $p_R, p_L \to 0$ with fixed ratio

$$q^2 = \frac{p_R}{p_L} \tag{12}$$

expressing the asymmetry in the hopping process. The continuous-time parameter τ (setting the hopping timescale) is obtained by taking the limit $t \to \infty$, keeping $\tau = t(p_R + p_L)$ fixed.

In the next step we want to specify the dynamics of this parallel update ASEP model in terms of the quantum Hamilton formalism. If we denote the first temporal step $\hat{T}_o$, the second one $\hat{T}_e$ and the total temporal evolution $\hat{T}$ we can then express the total time evolution as follows:

$$\hat{T} = \hat{T}_e \hat{T}_o. \tag{13}$$

The discrete operator $\hat{T}_o$ can be encoded in the quantum Hamiltonian form

$$\begin{aligned}\hat{T}_o &= \prod_{k=-L+1}^{L} \{1 - p_R[n_{2k-1}(1-n_{2k}) - s^+_{2k-1}s^-_{2k}] - p_L[(1-n_{2k-1})n_{2k} - s^-_{2k-1}s^+_{2k}]\} \\ &= \prod_{k=-L+1}^{L} \hat{T}_{o,(2k-1)} = \prod_{k=-L+1}^{L} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1-p_L & p_R & 0 \\ 0 & p_L & 1-p_R & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{2k-1,2k}\end{aligned} \tag{14}$$

where the n_k are the number operators giving the occupation number at site k and

$$s^+_k = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_k \qquad s^-_k = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_k \tag{15}$$

are spin ladder operators acting non-trivially on site k but as unit elements on all other sites, i.e., for any single-site operator A,

$$A_k = \mathbf{1} \otimes \cdots \mathbf{1} \otimes A \otimes \mathbf{1} \cdots \otimes \mathbf{1}. \tag{16}$$

One should stress that we connect particle occupancies with spins only for convenience. Analogously one can define $\hat{T}_e$, with the local $(2k-1, 2k)$ transfer matrix in (14) replaced by a similar $(2k, 2k+1)$ transfer matrix and $k \in [-L+1, L-1]$. It is easy to check that the stationary state of this chain has no correlations, i.e., is a product measure, but it requires two different densities for the odd and even sub-lattices, respectively [25]. We denote these sub-lattice densities by

$$\rho^A = \langle n_{2k-1} \rangle \qquad \text{and} \qquad \rho^B = \langle n_{2k} \rangle. \tag{17}$$

In vector notation such a product state may be written

$$\begin{aligned}|P^*\rangle &= \prod_{k=-L+1}^{L} \begin{pmatrix} 1-\rho^A & 0 \\ 0 & \rho^A \end{pmatrix}_{2k-1} \begin{pmatrix} 1-\rho^B & 0 \\ 0 & \rho^B \end{pmatrix}_{2k} |\vec{r}\rangle \\ &= [(1-\rho^A)(1-\rho^B)]^{2L} \prod_{k=-L+1}^{L} \hat{Z}^A_{2k-1} \hat{Z}^B_{2k} |\vec{r}\rangle\end{aligned} \tag{18}$$

with

$$\hat{Z}^{A/B} = \begin{pmatrix} 1 & 0 \\ 0 & z^{A/B} \end{pmatrix} \qquad \text{and} \qquad z^{A/B} = \frac{\rho^{A/B}}{1-\rho^{A/B}}. \tag{19}$$

Defining the local two-component vectors

$$|\rho^{A,B}\rangle = \begin{pmatrix} 1-\rho^{A,B} \\ \rho^{A,B} \end{pmatrix} \tag{20}$$

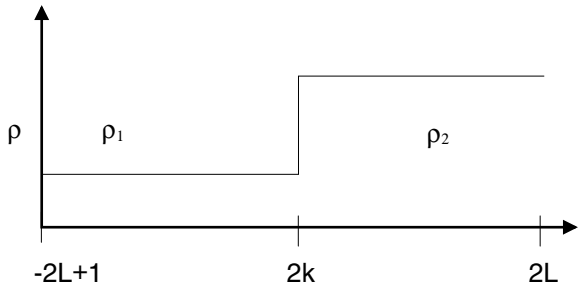

Figure 2. Schematic representation of the density profile in an upward shock at site $2k$.

the stationarity distribution may alternatively be written

$$|P^*\rangle = |\rho^A\rangle \otimes |\rho^B\rangle \cdots |\rho^A\rangle \otimes |\rho^B\rangle. \tag{21}$$

To prove the stationary element we note that the local hopping matrix T_k acting on this vector exchanges the A and B sub-lattice densities in a $(k, k+1)$ pair provided that they are related by

$$(1 - p_R)z^A = (1 - p_L)z^B. \tag{22}$$

With the sub-lattice update sequence chosen above, $\hat{T}_o$ interchanges all sub-lattice densities when acting on the stationary state, i.e. it shifts the density by one lattice unit. In the next step $\hat{T}_e$ shifts the sub-lattice densities again by unity (except in the boundary sites $-2L+1$ and $2L$ respectively), hence restoring the original bulk state. Neglecting the boundaries (or in the special case of periodic conditions which we do not consider here) the stationary element of the product state with arbitrary total density $\rho = \frac{1}{2}(\rho^A + \rho^B) \in [0, 1]$, but sub-lattice densities satisfying the constraint (22) is proved.

3.2. Definition of a shock

In this section we will calculate the temporal distribution for a family of shock initial states. Although we intend to carry out the computation in the thermodynamic limit we begin with a finite chain of $4L$ sites. The evolution of the system will be described by the transfer matrix $\hat{T}$ mentioned above in the description of the quantum Hamiltonian formalism.

Our shock at position $2k+1$ is defined in the following manner (figure 2): up to a position $2k$ the product measure on $\{0, 1\}$ has the density

$$\rho_1 = \tfrac{1}{2}(\rho_1^A + \rho_1^B) \tag{23}$$

whereas all other sites $\geqslant 2k+1$ have density

$$\rho_2 = \tfrac{1}{2}(\rho_2^A + \rho_2^B). \tag{24}$$

Notice that the individual sub-lattice densities $\rho_{1,2}^{A,B}$ are then fixed in each domain by (22). We call this measure a *shock measure* at $2k+1$ and denote it by μ_{2k+1}. Shocks at an even position $2k$ are defined as follows: up to site $2k-2$ the density is ρ_1. At site $2k-1$ $(2k)$ the density is ρ_1^A (ρ_2^B). At all other sites the density is ρ_2. The jump in the densities $\rho_{1,2}$ may be regarded as a domain wall connecting two stationary regions of the system. In order to have a *stable shock* which does not smear out in time we use the stability criterion of [6] which requires $\rho_1 < \rho_2$ for the ASEP discussed here.

It is convenient to represent the shock measure μ_k as a vector $|\mu_k\rangle$ in the Fock space. In this formalism it is a tensor product similar to the stationary product measure (18), but with two

different bulk particle densities (for details, see below). In terms of this vector we can state the main result of this paper which describes the time evolution of an initial shock measure under the action of the transfer matrix $\hat{T}$ (13). We find the measure at time t for a certain relation between the shock densities $\rho_{1,2}$ (specified below) as given by the linear combination

$$|\mu_k(t)\rangle = \sum_l \pi_l^k(t)|\mu_l\rangle. \tag{25}$$

The coefficients $\pi_l^k(t)$ calculated below can be interpreted as the transition probability of the shock to move from site k to site l after t time steps.

In order to obtain these transition probabilities and understand their physical origin we first show how a shock measure evolves after one time step, i.e., we calculate $\hat{T}|\mu_k(t)\rangle$. As an input we use the fact that when acting with $\hat{T}$ to the *left*, there is a family of observables $\hat{Q}_k$, indexed by the lattice site k, for which the resulting equations of motion form a closed set, i.e. without leading to an infinite hierachy of equations. This property is a result of the quantum group symmetry $U_q[SU(2)]$ of the process [13, 16]. In a series of technical steps (section 3.3) we determine two transformations $\hat{D}$, $\hat{V}$ which relate the transpose of the transformed transfer matrix to the original transfer matrix and which therefore allows us to turn the closed set of dynamical equations for the observables $\hat{Q}_k$ into a closed set of equations for unnormalized initial distributions. To this end one has to apply the transformation to the transpose of $\langle\vec{r}|\hat{Q}_k$. Normalizing the resulting distributions yields the shock measures. Putting everything together (section 3.4) then yields the desired result, i.e., the evolution of a shock measure after one time step. Since in the derivation of section 3.3 we have neglected the action of the transformations on the boundary we have to correct for this by taking the thermodynamic limit. This is discussed in a non-technical manner in section 3.5. We remark that for the continuous-time process studied in [14] the transformation is trivial and is not included. However, taking the thermodynamic limit remains necessary and is implemented in a mathematically rigorous manner.

3.3. Dynamics of the shock

First, we introduce a diagonal operator

$$\hat{Q}_k := \prod_{l=k}^{2L} \begin{pmatrix} 1 & 0 \\ 0 & q^2 \end{pmatrix}_l \equiv \prod_{l=k}^{2L} \Theta_l \tag{26}$$

(k may be even or odd) which is related to the shock as will be shown below. Let us start with one-time step evolution of $\hat{Q}_k$

$$\langle\hat{Q}_k(t+1)\rangle = \langle\vec{r}|\hat{Q}_k\tilde{T}\hat{V}^T|P(t)\rangle = \langle\vec{r}|\hat{Q}_k\tilde{T}_o\tilde{T}_e\hat{V}^T|P(t)\rangle \tag{27}$$

with the initial distribution $\hat{V}|P(t)\rangle$, and $\hat{V}$ is a diagonal operator. Here we used a slightly different stochastic transfer matrix $\tilde{T} = \tilde{T}_o\tilde{T}_e$ where compared to above we changed the update sequence and exchanged the hopping probabilities $p_R \Leftrightarrow p_L$. It is known from the quantum group symmetry ($U_q[SU(2)]$ with q as the asymmetry ratio (12)) that the time evolution of $\hat{Q}_k$ yields a closed set of equations in the site index k which can be interpreted as one-particle dynamics [13, 16]. Now we want to exploit this result by applying it to our original dynamics. Transposing the expectation value (27) yields

$$\langle P(0)|\hat{V}\tilde{T}_e^T\tilde{T}_o^T\hat{Q}_k|\vec{r}\rangle. \tag{28}$$

We want to choose $\hat{V}\hat{Q}_k$ such that $\hat{V}\hat{Q}_k|\vec{r}\rangle$ is a shock at position k which contains stationary regions in front of and behind the shock as defined above. Because $\hat{V}$ and $\hat{Q}_k$ (both diagonal) commute, $\hat{V}|\vec{r}\rangle$ should become a stationary state of the whole system, whereas $\hat{Q}_k$ fixes the

position where the density changes. Given the alternating density of the stationary state we may write $\hat{V} = \otimes_{k=-L+1}^{L}(\hat{V}^A \otimes \hat{V}^B)$ where $\hat{V}^{A,B}$ are diagonal 2×2 matrices and $\otimes$ denotes the tensor product. This determines the elements of $\hat{V}$ up to an irrelevant constant factor

$$\hat{V}^A \otimes \hat{V}^B = \hat{Z}^A \otimes \hat{Z}^B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & z^B & 0 & 0 \\ 0 & 0 & z^A & 0 \\ 0 & 0 & 0 & z^A z^B \end{pmatrix} \tag{29}$$

with

$$z^{A/B} = \frac{\rho^{A/B}}{1-\rho^{A/B}}. \tag{30}$$

Up to now the total chain has density ρ which we set without loss of generality to ρ_1. Starting from position k we want to create the density ρ_2 instead of ρ_1. To achieve this goal we may use the operator

$$\Theta_l = \begin{pmatrix} 1 & 0 \\ 0 & q^2 \end{pmatrix}_l. \tag{31}$$

Then the action of the operator Θ_l on a state $|\rho_1\rangle$ at one lattice site l is given by

$$\frac{1+z_1^{A/B}}{1+z_2^{A/B}}\Theta_l|(\rho_1^{A/B})_l\rangle = \frac{1}{1+z_2^{A/B}}\hat{Z}_2^{A/B}|r_l\rangle = |(\rho_2^{A/B})_l\rangle. \tag{32}$$

We see that on site l we generate a state with a different density defined by the constraint

$$q^2 = \frac{z_2^A}{z_1^A} = \frac{z_2^B}{z_1^B}. \tag{33}$$

By applying Θ_l to all sites of the chain larger than k, i.e. acting with $\hat{Q}_k$ on the product state $|\rho_1\rangle$, yields a state corresponding to a shock measure with shock densities $\rho_{1,2}^{A/B}$ related by (33). The operator $\hat{Q}_{2k+1}$ of the whole chain, ρ_2 beginning from $2k+1$, therefore may be written

$$\hat{Q}_{2k+1} = \mathbf{1}^{\otimes 2(L+k)} \otimes \left[\begin{pmatrix} 1 & 0 \\ 0 & \frac{z_2^A}{z_1^A} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & \frac{z_2^B}{z_1^B} \end{pmatrix}\right]^{\otimes(L-k)}. \tag{34}$$

The shock representation follows immediately (up to the normalization)

$$\hat{V}\,\hat{Q}_{2k+1} = (\hat{Z}_1^A \otimes \hat{Z}_1^B)^{\otimes(L+k)} \otimes (\hat{Z}_2^A \otimes \hat{Z}_2^B)^{\otimes(L-k)}. \tag{35}$$

Coming back to the time evolution of $\hat{Q}_k$ one continues computing and obtains

$$\langle P(0)|(\hat{V}\tilde{T}_e^T\tilde{T}_o^T\hat{V}^{-1})\hat{V}\,\hat{Q}_k|\vec{r}\rangle = \langle P(0)|(\hat{V}\tilde{T}_e^T\hat{X}^{-1})(\hat{X}\tilde{T}_o^T\hat{V}^{-1})\hat{V}\,\hat{Q}_k|\vec{r}\rangle \tag{36}$$

where $\hat{X}$ is a further diagonal matrix to be determined. Notice that the transpose matrices $\tilde{T}_e^T$ and $\tilde{T}_o^T$ are no longer stochastic. To retain stochastic matrices we require that

$$(\hat{V}\tilde{T}_e^T\hat{X}^{-1}) = \hat{T}_e \qquad \text{and} \qquad (\hat{X}\tilde{T}_o^T\hat{V}^{-1}) = \hat{T}_o. \tag{37}$$

Thus, we obtain the original transfer matrix (13) again. To determine $\hat{X}$ one applies the linear shift operator $\hat{D}$ to shift all operators from one sub-lattice to the other and get by means of (37)

$$\hat{D}\hat{V}\hat{D}^{-1} = \hat{X}. \tag{38}$$

To summarize, the matrices satisfy the relations

$$(\hat{V}\tilde{T}_e^T\hat{D}^{-1}\hat{V}^{-1}\hat{D}) = \hat{T}_e \qquad \text{and} \qquad (\hat{D}\hat{V}\hat{D}^{-1}\tilde{T}_o^T\hat{V}^{-1}) = \hat{T}_o. \tag{39}$$

Together with the condition of the stationary element, we recover from this relation the constraint (22) inside a domain (of course separately valid for each domain 1 and 2, that is the reason why we will call it the *intra-domain relation*).

In the next step we proceed with the shock as a wall separating two domains of stationary states with densities ρ_1 and ρ_2, respectively. Starting from the representation of the stationary state for $\hat{V}$ (29), $\hat{Q}_{2k+1}$ (34) and the requirement that $\hat{V}\hat{Q}_{2k+1}|\vec{r}\rangle$ should be a normalized shock the initial distribution for an odd-type shock at position $2k+1$ results in

$$\begin{aligned}|\mu_{2k+1}\rangle &= \hat{V}\hat{Q}_{2k+1}|\vec{r}\rangle \\ &= C^{-1}\left(\frac{(1+z_2^B)(1+z_2^A)}{(1+z_1^B)(1+z_1^A)}\right)^{L+k}(\hat{Z}_1^A)^{\hat{N}_{2k-1}}(\hat{Z}_1^B)^{\hat{N}_{2k}} \\ &\quad\times(\hat{Z}_2^A)^{\hat{N}_o-\hat{N}_{2k-1}}(\hat{Z}_2^B)^{\hat{N}_e-\hat{N}_{2k}}|\vec{r}\rangle \end{aligned} \tag{40}$$

where

$$C = ((1+z_2^B)(1+z_2^A))^{2L} \tag{41}$$

is the normalization and

$$\begin{aligned}\hat{N}_{2k-1} &= \sum_{i=-L+1}^{k} n_{2i-1} \qquad & \hat{N}_{2k} &= \sum_{i=-L+1}^{k} n_{2i} \\ \hat{N}_o &= \sum_{i=-L+1}^{L} n_{2i-1} \qquad & \hat{N}_e &= \sum_{i=-L+1}^{L} n_{2i}\end{aligned} \tag{42}$$

are sums of number operators. For an even-type shock at position $2k$ the distribution reads

$$|\mu_{2k}\rangle = (\hat{Z}_2^B)^{n_{2k}}(\hat{Z}_1^B)^{-n_{2k}}\frac{(1+z_1^B)}{(1+z_2^B)}|\mu_{2k+1}\rangle. \tag{43}$$

3.4. Shock dynamics as a one-particle equation

Taking the odd-position shock representation (40), it easy to see that in the first half-time step (odd sub-lattice) there is only an update inside the domains because no pair (ρ_1, ρ_2) exists inside the chain. Thus, the shock does not move. However, in the second half-time step (even sub-lattice) there is a sequence (ρ_1, ρ_2) at pair positions $2k, 2k+1$. To obtain shock distributions again and to conserve stationarity inside the domains (except at the boundaries which we consider later) there remain three possible sequences inside this pair after the temporal update. Taking these constraints into account the equation of motion $|\mu_{2k+1}(t+1)\rangle = \hat{T}_e\hat{T}_o|\mu_{2k+1}(t)\rangle$ leads to four equations

$$\hat{T}_e\hat{T}_o|\mu_{2k+1}(t)\rangle = \pi_R|\mu_{2k+2}(t)\rangle + \pi_L|\mu_{2k}(t)\rangle + \pi_S|\mu_{2k+1}(t)\rangle \tag{44}$$

for three coefficients π_L, π_S and π_R. This equation is correct up to the treatment of the boundary discussed below. Thus one can understand the many-particle motion of a shock as a discrete random walk of only one particle by identifying the position of the shock with the position of the random walker. Therefore we could reduce degrees of freedom without loss of relevant information. From (44) we read off the probabilities

$$\pi_R = p_R\frac{1+z_1^B}{1+z_2^B} \tag{45}$$

$$\pi_S = (1-p_L-p_R)\frac{1+z_2^A}{1+z_1^A}\frac{1+z_1^B}{1+z_2^B} \tag{46}$$

$$\pi_L = p_L\frac{1+z_2^A}{1+z_1^A} \tag{47}$$

by using the constraint (33) between the shock densities (which we denote *inter-domain relation* in contrast to the intra-domain relation (22)).

Notice that the shock position k is determined by the position where the second density starts, independently of the sub-lattice structure. For the even shock one obtains

$$\hat{T}|\mu_{2k}\rangle = \pi_S\pi_L|\mu_{2k-1}\rangle + \pi_S\pi_R|\mu_{2k+1}\rangle + (2\pi_L\pi_R + \pi_S)|\mu_{2k}\rangle + \pi_L^2|\mu_{2k-2}\rangle + \pi_R^2|\mu_{2k+2}\rangle. \quad (48)$$

The shock distribution turns into a linear combination of the same distributions with weights identical with the jump probabilities of the evolution of the discrete time random walk. By iterating the evolution equations (44) and (48) we arrive at the main result (25) of this paper with the transition probabilities (45)–(47) and the rules described above.

From these rules it is clear that the motion of a shock can be reformulated and understood as a random walk of a single particle with sub-lattice update according to the following updating scheme. In the first half-time step we consider only the even sub-lattice. If the particle is at position $2k$ then it moves with the probability π_L and π_R to the left and to the right respectively. In the second half-time step we shift to the odd sub-lattice and let the particle evolve in the same manner as in the first half-time step. This procedure leads immediately to the hopping rules (48). In the same manner one recovers (44) if there was a particle at site $2k+1$ at the beginning of the first half-step. The solution of this random walk problem yields the transition probabilities $\pi_l^k(t)$.

3.5. Boundary effects

The result of the previous subsection is the equation of motion which holds for the bulk, but with the incorrect consideration of the boundary (we regarded the finite chain with $4L$ sites). The next step is to remedy the influence of the boundary by taking the limit for L to infinity. Up to this point the ends are 'incorrectly' treated, i.e. after one time step we have the density ρ_B^1 instead of ρ_A^1 at the end point $-2L+1$ and the density ρ_A^2 instead of ρ_B^2 at the other end points $2L$, but the shock distribution is still properly normalized. With the proper treatment of the boundary equation (44) reads

$$\hat{T}|\mu_{2k+1}\rangle = \pi_S|\mu_{2k+1}\rangle_{-2L+1,2L} + \pi_L|\mu_{2k}\rangle_{-2L+1,2L} + \pi_R|\mu_{2k+2}\rangle_{-2L+1,2L} \quad (49)$$

where the indices mark the deviation at the boundary for the odd-type shock. For the even-type shock one obtains

$$\begin{aligned}\hat{T}|\mu_{2k}\rangle = {} & \pi_S\pi_L|\mu_{2k-1}\rangle_{-2L+1,2L} + \pi_S\pi_R|\mu_{2k+1}\rangle_{-2L+1,2L} \\ & +(2\pi_L\pi_R + \pi_S)|\mu_{2k}\rangle_{-2L+1,2L} + \pi_L^2|\mu_{2k-2}\rangle_{-2L+1,2L} + \pi_R^2|\mu_{2k+2}\rangle_{-2L+1,2L}. \quad (50)\end{aligned}$$

The disturbances of the boundary would evolve and finally destroy the shock distribution. However, this spreading of the disturbance takes place with a finite speed of two lattice units per time step. Thus, for $L \to \infty$ and finite time, there is always an infinite unaffected region around the shock position, i.e. we may conclude

$$\lim_{L\to\infty} |\mu_k(t)\rangle_{-2L+1,2L} = \lim_{L\to\infty} |\mu_k(t)\rangle \quad (51)$$

for all fixed number of time steps t.

Of course, the conservation of probability is still guaranteed because the boundary effects do not affect the normalization. We conclude that in the thermodynamic limit equations (44) and (48) are exact. The shock evolves into a linear combination of shock distributions if all constraints, i.e. the inter-domain relation (33) between the shock densities (resulting from the $U_q[SU(2)]$ symmetry) and the intra-domain relation (22) (for stationary states within the domains), are fulfilled.

4. Conclusions

Using the quantum algebra symmetry of the ASEP with sub-lattice parallel update as an input, we have obtained the time evolution of an initial shock distribution. Perhaps the most important observation is the possibility of the description of the collective many-body dynamics by a stochastic single-particle motion without having to resort to some approximation or scaling argument. The price we have to pay for obtaining the exact time-dependent shock measure is a constraint (33) on the shock densities which results from the underlying quantum algebra symmetry.

By analysing the properties of the associated random walk problem we can calculate the exact drift velocity and diffusion coefficient of the shock. The shock velocity v_S corresponds to the drift velocity of the random walk if we insert the transition probabilities π_S, π_R and π_L of (45)–(47) into (A.14). We obtain

$$\begin{aligned} v_S &= \frac{2(p_R - p_L)(1 - \rho_2^B - \rho_1^A)}{(1 - p_R) + (1 - p_L) + (p_R - p_L)(\rho_2^B - \rho_1^A)} \\ &= \frac{(p_R - p_L)(1 - \rho_2^B - \rho_1^A)}{\rho_2 - \rho_1}(\rho_2^A - \rho_1^B). \end{aligned} \tag{52}$$

If we take the current of both stationary domains [25]

$$j = p_R \rho^A (1 - \rho^B) - p_L \rho^B (1 - \rho^A) \tag{53}$$

and the total densities on both sides, equations (23) and (24), we can rewrite the shock velocity:

$$v_S = \frac{j_2 - j_1}{\rho_2 - \rho_1}. \tag{54}$$

It is clear that while (54) was derived directly only under the assumption that the constraint (33) holds, it must be generally valid. This is a simple consequence of mass conservation and reflects the more general principles of shock dynamics independent of the microscopic details and the update scheme. The parameter dependence of the shock velocity is shown in figure 3.

If we insert the transition probabilities (45)–(47) into the particle diffusion coefficient (A.19) we can compute the shock diffusion coefficient

$$D_S = \frac{2(p_R + p_L) + 2(p_R - p_L)(\rho_2^B - \rho_1^A)}{(1 - p_R) + (1 - p_L) + (p_R - p_L)(\rho_2^B - \rho_1^A)} \left[1 - \left(\frac{v_S}{2}\right)^2\right] \tag{55}$$

which represents the width of the shock distribution and thus gives a measure for its fluctuation. The hopping probability dependence of the diffusion constant is shown in figure 4. It is remarkable that the diffusion coefficient can also be expressed in terms of currents and densities of the shock domains. Using (53) one obtains

$$D_S = \frac{j_2 + j_1}{\rho_2 - \rho_1} \left[1 - \left(\frac{v_S}{2}\right)^2\right]. \tag{56}$$

We believe not only that the expression (54) for the drift velocity is generally valid, but also the expression (56). That is, if the constraint (33) is not satisfied and hence a single-particle picture is not strictly valid on the lattice scale, (56) should remain valid, even though we do not know of an underlying general principle. This expression for the diffusion coefficient is different from that of the time-continuous exclusion process [9, 10]. Thus it depends on the details of the stochastic dynamics. There is, however, an analogy to the time-continuous exclusion process insofar as in both models the shock dynamics have the same characteristic long-time properties as single particles in the respective processes, i.e. drift velocity and diffusion coefficient are the same for shock and particle respectively if one replaces the particle

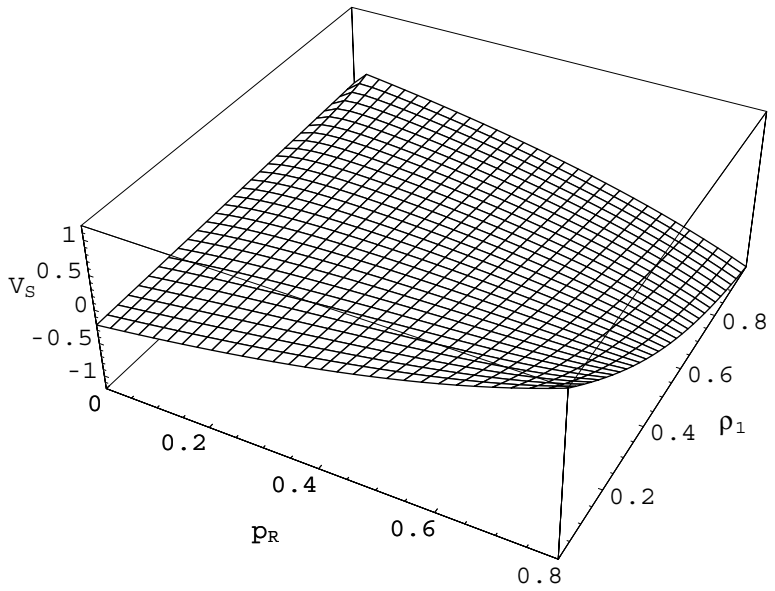

Figure 3. Shock velocity v_S as function of p_R and $\rho 1$ ($p_L = 0.2$, therefore $q = 0, \ldots, 2$).

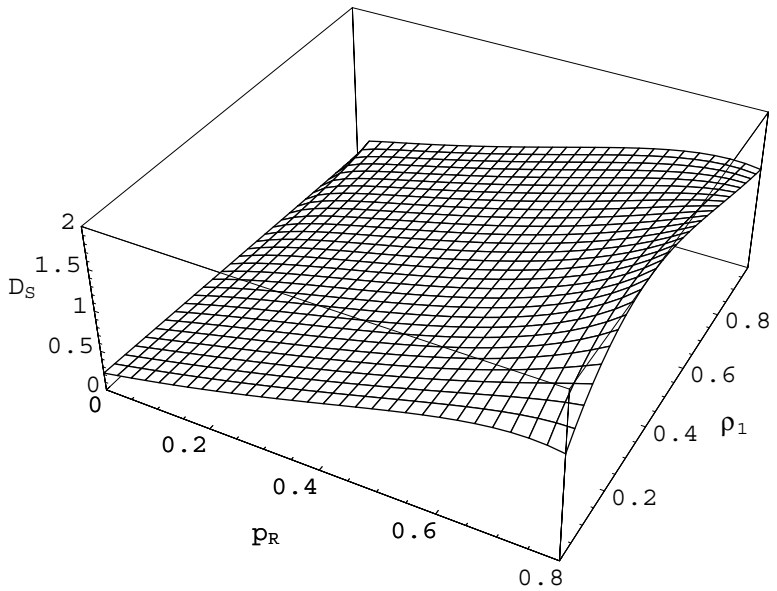

Figure 4. Shock diffusion constant D_S as function of p_R and $\rho 1$ ($p_L = 0.2$, therefore $q = 0, \ldots, 2$).

hopping rates (probabilities) by effective hopping rates (probabilities) for the shock. Since in the time-continuous exclusion process the expression of the shock diffusion coefficient in terms of the currents and densities is generally valid it seems plausible that this would remain true also for the present discrete-time realization of the exclusion process.

Appendix. Drift velocity and diffusion constant for the one-particle random walk

The shock $|\mu_k\rangle$ is labelled with the index expressing its position (k), which performs a random walk. We want to denote it for the following computation as a Fock space vector $|k\rangle$. From its random walk dynamics we may calculate its drift velocity and its diffusion constant which can be identified with the shock velocity and the shock diffusion constant.

Using the system of coupled equations (49) and (50) one can explicitly calculate the higher moments $\langle k^n(t)\rangle$

$$\langle k^n(t)\rangle = \sum_{k=-\infty}^{\infty} k^n P(k,t) = \langle k_e^n(t)\rangle + \langle k_o^n(t)\rangle \tag{A.1}$$

by means of the definition

$$\langle k_e^n(t)\rangle := \sum_{k=-\infty}^{\infty} (2k)^n P(2k,t) \qquad \text{and} \qquad \langle k_o^n(t)\rangle := \sum_{k=-\infty}^{\infty} (2k+1)^n P(2k+1,t). \tag{A.2}$$

These quantities are moments of the spatial probability distribution of the random walker. They lead to the drift velocity

$$v = \lim_{t\to\infty} (\langle k(t+1)\rangle - \langle k(t)\rangle) \tag{A.3}$$

and the diffusion constant

$$D = \lim_{t\to\infty} \langle (k(t+1) - \langle k(t+1)\rangle)^2\rangle - \langle (k(t) - \langle k(t)\rangle)^2\rangle. \tag{A.4}$$

To calculate these moments we write the master equation for the probabilities $P(k,t)$. This can be formally obtained by starting from the master equation (2) under consideration of the probability representation (4)

$$\begin{aligned}
\hat{T}|P(t)\rangle = \hat{T}\sum_l |l\rangle &= \hat{T}\sum_l P((2l,t)|2l\rangle + P(2l+1,t)|2l+1\rangle) \\
&= \sum_l \{[\pi_L^2 P(2l,t)]|2l-2\rangle + [\pi_L\pi_S P(2l,t)]|2l-1\rangle\} \\
&\quad + \sum_l [\pi_L P(2l+1,t) + \pi_S P(2l,t) + 2\pi_R\pi_L P(2l,t)]|2l\rangle \\
&\quad + \sum_l [\pi_S P(2l+1,t) + \pi_R\pi_S P(2l,t)]|2l+1\rangle \\
&\quad + \sum_l [\pi_R P(2l+1,t) + \pi_R^2 P(2l,t)]|2l+2\rangle.
\end{aligned} \tag{A.5}$$

We obtain the odd-type master equation (which, of course, may be found directly from the definition of the process)

$$\begin{aligned}
P(2k+1,t+1) &= \langle 2k+1|\hat{T}|P(t)\rangle \\
&= \pi_S P(2k+1,t) + \pi_L\pi_S P(2k+2,t) + \pi_R\pi_S P(2k,t)
\end{aligned} \tag{A.6}$$

if we apply the orthogonality of the states. Inserting the master equation into the odd part of the moments (A.2) yields

$$\begin{aligned}
\langle k_o^0(t+1)\rangle &= \sum_k P(2k+1,t+1) \\
&= \pi_S\langle k_o^0(t)\rangle + (1-\pi_S)\pi_S\langle k_e^0(t)\rangle
\end{aligned} \tag{A.7}$$

bearing the probability conservation $\pi_S + \pi_L + \pi_R = 1$ in mind.

In the case of the even-type dynamics one gets equivalently

$$\begin{aligned} P(2k,t+1) &= \langle 2k|\hat{T}|P(t)\rangle \\ &= (2\pi_L\pi_R+\pi_S)P(2k,t)+\pi_L P(2k+1,t)+\pi_R P(2k-1,t) \\ &\quad +\pi_L^2 P(2k+2,t)+\pi_R^2 P(2k-2,t). \end{aligned} \tag{A.8}$$

Taking the even part of (A.2) the master equation results in

$$\begin{aligned} \langle k_e^0(t+1)\rangle &= \sum_k P(2k,t+1) \\ &= (1-\pi_S)\langle k_o^0(t)\rangle + [(1-\pi_S)^2+\pi_S]\langle k_e^0(t)\rangle. \end{aligned} \tag{A.9}$$

Due to the conservation $\langle k_e^0(t)+k_e^0(t)\rangle = 1$ the equations (A.7) and (A.9) are not independent. Their stationary solution is given by

$$\langle k_e^0\rangle = \frac{1}{1+\pi_S} \qquad \text{and} \qquad \langle k_o^0\rangle = \frac{\pi_S}{1+\pi_S}. \tag{A.10}$$

This gives the stationary probability of finding the random walker (i.e. the shock position) on the even and odd sub-lattice, respectively.

To simplify the subsequent calculations we assume as the initial condition that the particle is sitting at an arbitrary position x on the odd lattice, i.e.

$$P(k,0) = \delta_{k,x}. \tag{A.11}$$

However, this initial assumption does not influence the asymptotic behaviour. One determines successively the higher moments from the known lower moments. Thus we get two coupled equations for the first moments:

$$\langle k_o^1(t+1)\rangle = \pi_S\langle k_o^1(t)\rangle + (1-\pi_S)\pi_S\langle k_e^1(t)\rangle + (\pi_R-\pi_L)\pi_S\langle k_e^0(t)\rangle \tag{A.12}$$

and

$$\begin{aligned} \langle k_e^1(t+1)\rangle &= (1-\pi_S)\langle k_o^1(t)\rangle + [(1-\pi_S)^2+\pi_S]\langle k_e^1(t)\rangle \\ &\quad +2(1-\pi_S)(\pi_R-\pi_L)\langle k_o^0(t)\rangle + (\pi_R-\pi_L)\langle k_e^0(t)\rangle. \end{aligned} \tag{A.13}$$

Solving this difference system under consideration of (A.10) and looking for the asymptotic limit of the particle drift velocity v (A.3) one finds

$$v = 2\frac{\pi_R-\pi_L}{1+\pi_S}. \tag{A.14}$$

If one interprets

$$\Pi_{R/L} = \frac{\pi_{R/L}}{1+\pi_S} \tag{A.15}$$

as an effective jump probability, v can be written as

$$v = 2(\Pi_R - \Pi_L). \tag{A.16}$$

To determine the diffusion constant we still need the second moments

$$\langle k_o^2(t+1)\rangle = \pi_S\langle k_o^2(t)\rangle + (1-\pi_S)\pi_S\langle k_e^2(t)\rangle + 2(\pi_R-\pi_L)\pi_S\langle k_e^1(t)\rangle + (1-\pi_S)\pi_S\langle k_e^0(t)\rangle \tag{A.17}$$

and

$$\begin{aligned} \langle k_e^2(t+1)\rangle &= (1-\pi_S)\langle k_o^2(t)\rangle + [(1-\pi_S)^2+\pi_S]\langle k_e^2(t)\rangle \\ &\quad +4(1-\pi_S)(\pi_R-\pi_L)\langle k_o^1(t)\rangle + 2(\pi_R-\pi_L)\langle k_e^1(t)\rangle \\ &\quad +(1-\pi_S)\langle k_o^0(t)\rangle + 2[(1-\pi_S)^2+(\pi_R-\pi_L)^2]\langle k_e^0(t)\rangle. \end{aligned} \tag{A.18}$$

Computing this second difference equation system using (A.10) and the results of the first difference equation system (A.12), (A.13) we get the asymptotic limit of the particle diffusion constant D (A.4)

$$D = 2\frac{1-\pi_S}{1+\pi_S}\left[1-\left(\frac{v}{2}\right)^2\right] \tag{A.19}$$

using the velocity (A.14). In terms of the effective jump probabilities one has

$$D = 2(\Pi_R + \Pi_L)[1-(\Pi_R - \Pi_L)^2]. \tag{A.20}$$

We note that these expressions for the drift velocity and the diffusion coefficient are the same as those for a single exclusion particle with the sub-lattice dynamics of the exclusion process described above. Even though the microscopic dynamics of a single exclusion particle are different from the random walk discussed here the long-time properties are identical.

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