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Cellular automaton model for molecular traffic jams

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Abstract. We consider the time evolution of an exactly solvable cellular automaton with random initial conditions both in the large-scale hydrodynamic limit and on the microscopic level. This model is a version of the totally asymmetric simple exclusion process with sublattice parallel update and thus may serve as a model for studying traffic jams in systems of self-driven particles. We study the emergence of shocks from the microscopic dynamics of the model. In particular, we introduce shock measures whose time evolution we can compute explicitly, both in the thermodynamic limit and for open boundaries where a boundary-induced phase transition driven by the motion of a shock occurs. The motion of the shock, which results from the collective dynamics of the exclusion particles, is a random walk with an internal degree of freedom that determines the jump direction. This type of hopping dynamics is reminiscent of some transport phenomena in biological systems.

Keywords: cellular automata, driven diffusive systems (theory)

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1. Introduction

In the framework of a macroscopic description of many-body systems far from thermal equilibrium one is often faced with a scalar conservation law of the form

$$\frac{\partial}{\partial \tau} \rho + \frac{\partial}{\partial x} j = 0 \quad (1)$$

where j is the current given as a function of the time-dependent local density $\rho \equiv \rho(x, \tau)$. Such a partial differential equation is known to emerge, for example, as the large-scale behaviour of microscopic models of stochastic-driven interacting particles such as the well-known asymmetric simple exclusion process (ASEP) [2]–[4]. For nonlinear current-density relations $j(\rho)$ solutions to (1) may have discontinuities which are known as shocks [1]. It is by now well understood that macroscopic shock solutions of (1) correspond to traffic jams on the microscopic scale which are ubiquitous in systems of self-driven particles such as molecular motors in cells, vehicular highway traffic, or pedestrian dynamics (see [5]–[8] specifically for the important case of molecular motors and [9] for an up-to-date and comprehensive general overview). It is therefore of considerable interest to study the microscopic properties of shocks in detail.

So far most investigations of the microscopic structure of shocks have focused on stochastic interacting particle systems. Work on the ASEP has revealed very detailed

information about the microscopic shock structure [10]–[14], [44], [15]–[18]. The main tools in these investigations are the introduction of a second-class particle that serves as the microscopic definition of a shock and of shock measures which are measures that connect two stationary regimes of different constant density and thus correspond to step function density profiles on the macroscopic scale. Recently we have extended these ideas to study an exclusion process with deterministic bulk dynamics [19], the so-called cellular automaton 184 (CA 184) defined on the infinite integer lattice $\mathbb{Z}$ [20]. This model is a discrete time version of the totally asymmetric simple exclusion process (TASEP) where particles jump only in one direction, subject to a parallel update rule. Random initial conditions in CA 184 have been known for some time to lead to non-trivial relaxation dynamics [21, 22]. We have shown that interesting dynamics appear also for shock measures for which we have defined a microscopic shock position and studied the structure of the shock [19].

It is the aim of this work to go beyond the approach of [19] and to study shocks in deterministic CA by considering a finite system with open boundaries which is expected to exhibit boundary-induced phase transitions [23, 24]. To this end we slightly modify the updating rules of CA 184 in a way that leaves the macroscopic behaviour (1) essentially unchanged, but facilitates the treatment of the microscopic properties. We shall consider a CA that corresponds to a TASEP with sublattice update. For open boundaries the stationary distribution of this model exhibits a boundary-induced phase transition between a free-flow low-density phase and a congested high-density phase [25]. Here we introduce a microscopic definition of the shock position, establish various microscopic properties of the shock, and use these results to study the dynamics of the non-equilibrium first-order phase transition in terms of the dynamics of a shock, which corresponds to a traffic jam of particles on the lattice.

This paper is organized in the following way. In the next section we introduce the model and review some of its stationary properties. We also outline the large-scale behaviour which is given by an equation of the form (1). In section 3 we define a microscopic shock and explore some of its fundamental properties. In section 4 we study the dynamics of the phase transition. In section 5 we summarize our results and draw some conclusions.

2. Cellular automaton with sublattice update

2.1. Definition of the model

In this cellular automaton, which describes driven ballistic motion of particles with hard-core repulsion, each site k on the integer lattice $\mathbb{Z}$ is either occupied by a particle or empty. We denote the occupation number at time step t by $\eta_t(k) \in \{0, 1\}$. Each update of the discrete time dynamics consists of two steps. First all even–odd pairs of sites $(2k, 2k + 1)$ are updated such that in each pair a particle on site $2k$ jumps to site $2k + 1$ provided that $2k + 1$ was empty. Otherwise nothing changes. Therefore at the intermediate time t'

$$\begin{aligned}\eta_{t'}(2k) &= \eta_t(2k)\eta_t(2k + 1) \\ \eta_{t'}(2k + 1) &= \eta_t(2k) + \eta_t(2k + 1) - \eta_t(2k)\eta_t(2k + 1).\end{aligned}\tag{2}$$

In the second step the pairing is shifted by one lattice unit and each pair $(2k - 1, 2k)$ is updated with the same jump rule.

In a finite system with L sites (where L is even) the first step is applied only to the bulk pairs $(2, 3), \dots, (L-2, L-1)$. The boundary sites 1 and L are updated as follows: on site 1 a particle is injected with probability α if it was vacant. Otherwise nothing changes. On site L a particle is removed with probability β if it was occupied. Otherwise nothing changes. The boundary update attempts occur independently and we have

$$\begin{aligned} \eta_{t'}(1) &= 1 && \text{with probability } \eta_t(1) + \alpha(1 - \eta_t(1)) \\ \eta_{t'}(1) &= 0 && \text{with probability } (1 - \alpha)(1 - \eta_t(1)) \\ \eta_{t'}(L) &= 1 && \text{with probability } (1 - \beta)\eta_t(L) \\ \eta_{t'}(L) &= 0 && \text{with probability } 1 - (1 - \beta)\eta_t(L). \end{aligned} \quad (3)$$

Schematically we can represent the bulk update in each pair as follows

$$\begin{aligned} 00 &\rightarrow 00 & 0A &\rightarrow 0A \\ A0 &\rightarrow 0A & AA &\rightarrow AA \end{aligned} \quad (4)$$

where A denotes a particle and 0 a vacant site. It is convenient to write update rules only for those configurations that undergo a change, i.e. we may simply write

$$A0 \rightarrow 0A. \quad (5)$$

For the boundaries we have the update rules

$$\begin{aligned} \text{Site 1: } 0 &\rightarrow A && \text{with probability } \alpha \\ \text{Site } L: A &\rightarrow 0 && \text{with probability } \beta. \end{aligned} \quad (6)$$

The boundary occupations remain unchanged with the respective complementary probabilities $1 - \alpha, 1 - \beta$. Owing to the similarity with the original cellular automaton CA 184, where all particles are updated in parallel in one time step, we shall refer to the present lattice gas model as sublattice CA 184 (slCA184).

The Markovian time evolution of the process can be encoded in a transfer matrix which for a periodic chain of L sites (L even) is of the form [25, 26]

$$T = \prod_{j=1}^{L/2} T_{2j-1} \cdot \prod_{j=1}^{L/2} T_{2j} = T^{\text{odd}} T^{\text{even}}. \quad (7)$$

The local matrices T_j act non-trivially on sites j and $j+1$, on all other sites they act as unit operators. For an explicit representation we choose a spin-1/2 tensor basis where spin down at site j represents a particle (up-pointing arrow) and spin up a hole (down-pointing arrow). With the Pauli matrices $\sigma^{x,y,z}$ the matrix $\tau_j = (1 - \sigma_j^z)/2$ is the projection operator on particles on site j , $\sigma_j = (1 + \sigma_j^z)/2$ is the projector on holes and $s_j^\pm = (\sigma_j^x \pm i\sigma_j^y)/2$ create (s_j^-) and annihilate (s_j^+) particles respectively. This leads to

$$T_j = 1 + s_j^+ s_{j+1}^- - \tau_j \sigma_{j+1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{j,j+1}. \quad (8)$$

For open boundaries with injection of particles on site 1 and removal of particles on site L the local transfer matrix T_L acting on sites L and 1 is given by

$$T_L = (1 + \alpha(s_1^- - \sigma_1))(1 + \beta(s_L^+ - \tau_L)) \\ = \begin{pmatrix} 1 - \alpha & 0 & \beta(1 - \alpha) & 0 \\ \alpha & 1 & \alpha\beta & \beta \\ 0 & 0 & (1 - \alpha)(1 - \beta) & 0 \\ 0 & 0 & \alpha(1 - \beta) & 1 - \beta \end{pmatrix}_{L,1}. \quad (9)$$

The product form of T_L reflects the independence of injection and removal of particles at the two boundary sites.

2.2. Review of stationary properties

2.2.1. Infinite system. Let a particle distribution on $\mathbb{Z}$ be translation invariant (i.e. the distribution does not change, if it is shifted along $\mathbb{Z}$) and let it either have no particles on odd sites (and hence have no neighbouring particles) or have no vacancies on even sites (and hence have no neighbouring vacancies). Then, in both cases, this distribution is also time invariant both for CA184 and slCA184. We shall refer to time-invariant distributions as stationary distributions. Indeed, the following stationary properties of slCA184 are very similar to those of CA184 and our discussion follows largely the corresponding discussion in [19].

The particle density is defined by the space average

$$\rho = \lim_{L \rightarrow \infty} \frac{1}{2L} \sum_{k=-L+1}^L \eta_t(k). \quad (10)$$

Evidently, in the first case (no particles on odd sites) the particle density in the system is $\rho \leq 1/2$, while in the absence of vacancies on even sites one has $\rho \geq 1/2$. At stationary particle densities up to $1/2$ the system is said to be in the free-flow phase since according to (2) one has $\eta_{t+1}(k+2) = \eta_t(k)$, i.e. each particle moves two lattice units at each time step due to the absence of particle pairs. At densities larger than $1/2$ the system is said to be in the congested phase, since in any large enough region there are always some particles that cannot move in a given time step. Here in each step each vacancy moves two lattice units to the left. At density exactly equal to $1/2$, the stationary particle arrangement is trivial; this is the ordered configuration where particles on even sites and vacancies on odd sites alternate. Notice that because of particle conservation the density (10) is time independent for any microscopic configuration η .

Let us denote by $j(\rho)$ the particle current in a stationary distribution with particle density ρ , i.e. the expected number of particles crossing an arbitrary bond in one time step. We have

$$j(\rho) = \begin{cases} 2\rho & \text{if } \rho \leq 1/2 \\ 2(1 - \rho) & \text{if } \rho \geq 1/2. \end{cases} \quad (11)$$

This current-density relation, called a fundamental diagram in traffic engineering, determines the hydrodynamic behaviour (1) of the model, see below. Notice that the current-density relation (11) is the same as for CA184, except for a trivial factor of 2

which comes from our choice of time unit (two single update steps constitute one complete time step).

In order to prove (11) we first introduce for a particular initial configuration η_0 the time-integrated current $J_T(k) = \sum_{t=1}^T m_t(k)$ where $m_t(k)$ (taking values 0 or 1) is the number of particles that have crossed the bond $k, k+1$ at time step t , starting from a configuration η_0 . Clearly $J_T(k)$ is a fluctuating quantity whose distribution is completely determined by η_0 , unlike in the case of stochastic dynamics, which generate non-trivial universality classes of current distributions [27]–[33]. By the law of large numbers we obtain from the time-integrated current the average current

$$\tilde{j}_k = \lim_{T \rightarrow \infty} \frac{1}{T} J_T(k) \quad (12)$$

if the law of large numbers holds for the particle numbers $\eta_t(k)$ independently of k , i.e. one has for all $k \in \mathbb{Z}$

$$\rho = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{i=k-L+1}^k \eta(i). \quad (13)$$

If the configuration is taken from a stationary measure, i.e. it has no particle blocks ($\rho \leq 1/2$) or no vacancy blocks ($\rho \geq 1/2$) then $\tilde{j}_k = j(\rho)$. This is the situation that we shall encounter and therefore we do not distinguish between the two currents, unless necessary.

Clearly, the slCA184 is highly non-ergodic, since any arrangement of particles without neighbouring pairs of particles or vacancies gives rise to a stationary distribution. A special family of stationary distributions results as the deterministic limit of the random version of slCA184 where the same hopping rules are applied except that particles jump with probability p rather than deterministically. It follows from the work of [34, 35] that the unique family of time and translation-invariant measures of this process are Bernoulli product measures with alternating sublattice densities $\rho_{2k} = \rho_e$, $\rho_{2k+1} = \rho_o$ such that

$$\rho_o = \frac{(1-p)\rho_e}{1-\rho_e+(1-p)\rho_e}. \quad (14)$$

The total density is then $\rho = (\rho_e + \rho_o)/2$. In the limit $p \rightarrow 1$ these measures converge to measures of the kind described above, but with the special feature that for $\rho \leq 1/2$ one has $\rho_e = 2\rho$ and $\rho_o = 0$ while for $\rho \geq 1/2$ one has $\rho_e = 1 - 2\rho$ and $\rho_o = 1$. Consequently, for $\rho \leq 1/2$ the number v of vacancies on even sites between consecutive particles at even positions $2k_i, 2k_{i+1}$ is a geometrically distributed random variable with parameter 2ρ , i.e. $\text{Prob}[v = k] = 2\rho(1 - 2\rho)^k$. Likewise, for $\rho \geq 1/2$, the number of particles on odd sites between vacancies on odd sites is geometrically distributed with parameter $1 - 2\rho$.

2.2.2. Semi-infinite open system. The stationary measures introduced above arise also in a different interesting context, namely in a semi-infinite system with open boundary conditions. To set the stage, consider the non-negative ‘semi-line’ of $\mathbb{Z}$, that is, the set $\mathbb{N}_0 = \{0, 1, 2, \dots\}$. Let us postulate that all these sites are empty at time 0. Let us insert particles at time $1, 2, \dots$ at the left boundary site 0 by the following rule: if at time t there is no particle at 0, then we put a particle at 0 at time $t+1$ with the probability α , independently of any previous injection event, otherwise, we do not put a particle at

time $t + 1$. As time tends to infinity, the distribution of inserted particles is the same as if we constructed the particle distribution on $\mathbb{Z}$ in accordance to the geometric process described above, and then take its restriction to $\mathbb{N}_0$. The total density is $\rho = \alpha/2$.

Likewise one may study an open right boundary, i.e. the slCA184 dynamics on the left semi-line $\{\dots, L-2, L-1, L\}$ with boundary processes defined as follows: if at time t there is a particle at L , then we remove this particle at L at time $t + 1$ with the probability β , otherwise, the particle stays at L at time $t + 1$. If initially the left semi-line was completely filled with particles then effectively vacancies travelling to the left enter the system at its right boundary. As a result the distribution of particles tends to the geometric distribution as time diverges. If one takes the restriction of the geometric distribution on the left semi-line as the initial distribution the process is stationary. The total density is $\rho = 1 - \beta/2$.

2.2.3. Open boundary conditions. The stationary distribution for a finite system with open boundary conditions as defined above was first studied in [25] where rigorous results for the current and the density profile were obtained by solving recursion relations. These results were later reproduced in [36] using a different method, namely the matrix product ansatz [37]. We mention the following properties of the stationary distribution.

For $\alpha \neq \beta$ the density profile, i.e. the expected density $\rho_k = \langle \eta_k \rangle$ as a function of space, is essentially constant in the bulk, with corrections that decay exponentially in the (lattice) distance from the boundary. Hence there is a boundary layer of microscopic width. Moreover, due to the sublattice update there is an alternating sublattice structure in the density profile. Specifically, for $\alpha < \beta$ the bulk density is α on even sites and 0 on odd sites. There is a boundary layer at the right edge of the system. The stationary current is $j = \alpha = 2\rho$ where ρ is the total bulk density. For $\alpha > \beta$ the bulk density is $1 - \beta$ on odd sites and 1 on even sites. There is a boundary layer at the left edge of the system. The stationary current is $j = \beta = 2(1 - \rho)$.

This shows that there is a boundary-induced first-order phase transition along the line $\alpha = \beta$ where the bulk density has a jump discontinuity. As the phase transition line is approached, the width of the boundary layer diverges. Along the phase transition line the density profile is linear on both sublattices. According to the arguments of [23, 24] this is the signature of a shock-driven phase transition. One postulates that the two boundaries mimic boundary reservoirs with constant densities ρ_L, ρ_R of virtual reservoir particles and that a shock profile with a jump discontinuity connects the boundary densities. Because of mass conservation, a shock between densities ρ_1, ρ_2 moves with velocity

$$v_s = \frac{j(\rho_1) - j(\rho_2)}{\rho_1 - \rho_2}. \quad (15)$$

For the present model, $\rho_1 = \rho_L = \alpha/2$ and $\rho_2 = \rho_R = 1 - \beta/2$. Then in the low-density phase the shock has positive velocity and is thus driven to the right edge of the system where it remains localized, leaving the bulk at density $\rho = \rho_L < 1/2$. In the high-density phase the shock has negative velocity and is thus driven to the left edge of the system, leaving the bulk at density $\rho = \rho_R > 1/2$. Within this theory of boundary-induced phase transitions the boundary layers are the microscopic signature of two effects, small fluctuations of the shock position, which is argued to be microscopically sharp, and boundary correlations. At the phase transition line the shock velocity is zero,

but fluctuations are expected to lead to an unbiased random motion, leaving the shock everywhere with equal probability in a stationary measure. This then explains the linear density profile. The exact results of section 3 will be used to probe these theoretical predictions, identify the random motion of the shock and determine the origin of the structure of the boundary layer.

2.3. Large-scale behaviour

So far the lattice spacing has been implicitly set to unity. In order to study hydrodynamic scaling we introduce a lattice spacing a and study the model under Eulerian scaling $a \rightarrow 0$, with rescaled macroscopic space and time coordinates $x = ka$, $\tau = ta$. Particle conservation and local stationarity suggests that the large-scale behaviour of slCA184 is then governed by the hydrodynamic equation

$$\frac{\partial}{\partial \tau} \rho + v_c \frac{\partial}{\partial x} \rho = 0 \quad (16)$$

where j is the current given as a function of the local coarse-grained density ρ by (11) and

$$v_c(\rho) = \frac{d}{d\rho} j(\rho) \quad (17)$$

is the collective velocity. We remark that our approach to studying the relation between microscopic dynamics and macroscopic behaviour, which is in the spirit of [38], is very different from the route taken in [39] for CA 184 where a discrete difference equation is taken as the starting point from which both a continuum equation and the cellular automaton dynamics are derived as some limiting case.

We obtain as the scaling limit for slCA 184

$$\frac{\partial}{\partial \tau} \rho = \begin{cases} 2 \frac{\partial}{\partial x} \rho & \text{if } \rho < 1/2 \\ -2 \frac{\partial}{\partial x} \rho & \text{if } \rho > 1/2. \end{cases} \quad (18)$$

Clearly, any constant density profile is a (trivial) solution of this equation. Moreover, as long as initially the local density is everywhere below or above $1/2$, the initial density profile travels with fixed velocity ± 1 , but remains unchanged in shape. This includes shock profiles which are initially step functions of the form

$$\rho_0(x) := \rho(x, 0) = \begin{cases} \rho_1 & \text{if } x < x_0 \\ \rho_2 & \text{if } x > x_0 \end{cases} \quad (19)$$

with $\rho_1 < \rho_2$. If both ρ_1 and ρ_2 are below (above) $1/2$ then the shock will travel with speed $v_s = 2$ ($v_s = -2$). The macroscopic shock position at time τ is then given by $x_s(\tau) = x_0 \pm \tau$. Notice that this result is already clear from the microscopic dynamics on the lattice scale since at macroscopic timescales any domain that was initially finite (on lattice scale) and non-stationary will have relaxed into a locally stationary state and hence under the condition that both ρ_1 and ρ_2 are below or above $1/2$ we are dealing with a configuration in which indeed all particles (or vacancies) travel ballistically with speed ± 2 .

The situation is somewhat more intricate if one of the densities in an initial step profile is below $1/2$, while the other is above one half. Consider first $\rho_1 < 1/2$ and $\rho_2 > 1/2$. According to the Lax criterion for the existence of shocks [1] one expects shock solutions. In particular, the initial step function remains unchanged in shape and the macroscopic shock travels with speed (15). Notice that $v_s \rightarrow 2$ as $\rho_2 \rightarrow 1/2$ and $v_s \rightarrow -2$ as $\rho_1 \rightarrow 1/2$. This suggests that the discussion in the previous paragraph may be extended to initial profiles that are not everywhere strictly below or above $1/2$, but satisfy the less stringent inequality $\rho_0(x) \leq 1/2$ or $\rho_0(x) \geq 1/2$ for all x .

Next we consider an initial downward step with $\rho_1 > 1/2$ and $\rho_2 < 1/2$ which does not satisfy the Lax criterion for stable shocks. In lattice gases with stochastic dynamics one expects on the macroscopic scale the evolution of rarefaction waves from initial conditions with jump discontinuities that do not correspond to the microscopically stable shocks. These rarefaction waves are scaling solutions $\rho(u)$ with the scaling variable $u = x/\tau$, obtained from the hydrodynamic equation (16) as solutions of the implicit equation $u = v_c(\rho)$. Since the current (11) as a function of the density is piece-wise linear and therefore has a discontinuous piece-wise constant derivative, this method is not well defined for our problem.

In order to study this problem for slCA184 we take a direct microscopic approach and consider two stationary distributions on $\mathbb{Z}$ with the respective densities ρ_1 and ρ_2 such that $\rho_2 < \rho_1$. From these we construct a new distribution by taking the restriction on $(-\infty, k_0]$ of the first one, and the restriction on $[k_0 + 1, +\infty)$ of the other one, where k_0 is an odd site. It follows directly from the definition of the dynamics that particles at positions $> k_0$ do not interact and move ballistically with speed 2. Hence they may be completely ignored and without loss of generality we can set $\rho_2 = 0$ for investigating what happens to the step. Notice that by construction of the shock measure all odd sites $\leq k_0$ are occupied by a particle. Next we realize that the microscopic dynamics imply that the maximum output of particles from a given site is at most one per time unit and that this maximum is reached for a time interval of length s if and only if there are at least s particles on even sites to the left of k_0 . For the initial configuration considered here $s = \infty$ and hence in each time step a particle is injected into the empty region $> k_0$. Hence inside that region a locally stationary domain with density $1/2$ grows with speed 2. Coming back to the original initial state this domain is followed by the initial domain of density $\rho_2 < 1/2$. Applying similar arguments (in terms of vacancies travelling to the left) to the region $< k_0$ one finds that also there a locally stationary domain with density $1/2$ develops and spreads with speed -2 to the left. There it connects to a region with original density $\rho_1 > 1/2$.

Therefore on the macroscopic scale two consecutive stable down step with densities (ρ_1, ρ^*) , (ρ^*, ρ_2) arise, with intermediate particle density $\rho^* = 1/2$. Macroscopic mass conservation gives the propagation speed of these discontinuities according to (15) (where $\rho_2 = 1/2$ for the first step and $\rho_1 = 1/2$ for the second step).

3. Microscopic properties of the shock

We stress that step discontinuities where $\rho_2 < \rho_1$ do not satisfy the Lax criterion for stable shocks and we shall not regard them as shocks. Indeed, the evolution of such steps, starting from two stationary branches with densities $\rho_{1,2}$, is completely described above

even on the microscopic level. The problem of interest that remains and is studied in this section is the existence and dynamics of a well-defined microscopic position of a shock in a genuine shock initial state where $\rho_2 > \rho_1$.

In order to attack this problem we first introduce in the spirit of [11] second-class particles, denoted B . A second-class particle is updated like a first-class particle when there is no first-class particle inside a pair of sites. In the presence of a first-class particle it behaves like a vacancy. The corresponding jumps can be represented schematically as

$$B0 \rightarrow 0B \quad AB \rightarrow BA. \quad (20)$$

The structure $T = T^{\text{odd}}T^{\text{even}}$ of the transfer matrix for the time evolution of this extended process remains unchanged. The only difference is in the representation of the local transfer matrix T_j for neighbouring pairs of sites which becomes a 9×9 matrix owing to the fact that now each site can be in three states, namely vacant, occupied by a first-class particle, or occupied by a second-class particle. A natural choice of basis for these three states is

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |A\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |B\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (21)$$

Writing down T_j in the corresponding tensor basis is then straightforward.

3.1. Shock measures

Consider now shock measures which are defined as follows. With probability one there is a second-class particle located at some lattice position k . At all other sites the measure is stationary with density $\rho_1 \leq 1/2$ of first-class particles to the left of the (single) second-class particle and stationary with density $\rho_2 \geq 1/2$ of first-class particles to the right of the second-class particle. We shall consider the position of the second-class particle as the microscopic shock position. According to the sublattice structure of the invariant measure one puts on all even (odd) sites to the left of the second-class particle a first-class particle with probability $\alpha = \rho_1/2$ (probability zero), independently of each other. All odd (even) sites to the right of the second-class particle have a vacancy with probability $\beta = (1 - \rho_2)/2$ (probability zero), independently of each other. Depending on whether the shock position is even or odd, this construction defines two families of shock measures of product form which in the basis defined above are represented by the tensor vectors

$$|\mu_{2k-1}\rangle = \cdots |0\rangle \otimes |\alpha\rangle \otimes |0\rangle \otimes |\alpha\rangle \otimes |B\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \otimes |\gamma\rangle \cdots \quad (22)$$

$$|\mu_{2k}\rangle = \cdots |0\rangle \otimes |\alpha\rangle \otimes |0\rangle \otimes |B\rangle \otimes |\gamma\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \otimes |\gamma\rangle \cdots \quad (23)$$

where $\gamma = 1 - \beta$ and

$$|p\rangle = \begin{pmatrix} 1-p \\ p \\ 0 \end{pmatrix} = (1-p)|0\rangle + p|A\rangle \quad (24)$$

represents occupancy of a site by a first-class particle with probability p . The site index in the measure denotes the location of the second-class particle basis vector $|B\rangle$ in the tensor product.

In order to study the time evolution of these shock measures we decompose the marginal distribution next to the second-class particles as follows

$$|\mu_{2k-1}\rangle = (1 - \alpha) \cdots |\alpha\rangle \otimes |0\rangle \otimes |0\rangle \otimes |B\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \cdots \\ + \alpha \cdots |\alpha\rangle \otimes |0\rangle \otimes |A\rangle \otimes |B\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \cdots \quad (25)$$

$$|\mu_{2k}\rangle = \beta \cdots |\alpha\rangle \otimes |0\rangle \otimes |B\rangle \otimes |0\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \cdots \\ + (1 - \beta) \cdots |\alpha\rangle \otimes |0\rangle \otimes |B\rangle \otimes |A\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \cdots \quad (26)$$

(For the odd site index we have decomposed the marginal corresponding to left neighbouring site $2k - 2$ and for even site index we have decomposed the marginal corresponding to right neighbouring site $2k + 1$.) Applying the evolution rules we thus find

$$T|\mu_{2k-1}\rangle = \alpha^2 |\mu_{2k-3}\rangle + \alpha(1 - \alpha) |\mu_{2k-2}\rangle + (1 - \alpha)(1 - \beta) |\mu_{2k-1}\rangle + \beta(1 - \alpha) |\mu_{2k}\rangle \quad (27)$$

$$T|\mu_{2k}\rangle = \beta^2 |\mu_{2k+2}\rangle + \beta(1 - \beta) |\mu_{2k+1}\rangle + (1 - \alpha)(1 - \beta) |\mu_{2k}\rangle + \alpha(1 - \beta) |\mu_{2k-1}\rangle. \quad (28)$$

Interestingly these are the evolution rules for a partially asymmetric random walk that evolves under the sublattice dynamics of slCA184, hopping with probability β to the right when the walker is on an even site and with probability α to the left when the walker is on an odd site.

This closure of the time evolution on the set of shock measures is rather remarkable. It implies that we may regard the microscopic shock position as a random variable $X(t)$ such that the shock position performs a single-particle sublattice random walk with partially asymmetric transition probabilities determined by the particle densities in the two branches of the shock. Moreover, the microscopic structure of the shock as seen from the second-class particles remains unchanged for all times. We have for the conditional probability of finding a first class at a distance n from the location $X(t)$ second-class particle

$$\rho_{\text{cond}}^{\text{odd}}(n, t) := \text{Prob}[\tau_{k+n} = 1 | X(t) = k \text{ odd}] = \begin{cases} 1 & n > 0 \text{ odd} \\ 1 - \beta & n > 0 \text{ even} \\ \alpha & n < 0 \text{ odd} \\ 0 & n < 0 \text{ even} \end{cases} \quad (29)$$

$$\rho_{\text{cond}}^{\text{even}}(n, t) := \text{Prob}[\tau_{k+n} = 1 | X(t) = k \text{ even}] = \begin{cases} 1 & n > 0 \text{ even} \\ 1 - \beta & n > 0 \text{ odd} \\ \alpha & n < 0 \text{ even} \\ 0 & n < 0 \text{ odd} \end{cases} \quad (30)$$

All conditional correlations between first-class particles are independent of time and factorize.

3.2. Shock motion

We define $P_k(t) := \text{Prob}[X(t) = k]$ as the probability of finding the shock position at time t on site k . The forward evolution rules (27), (28) imply the following master equation

$$P_{2k-1}(t+1) = \alpha^2 P_{2k+1}(t) + \alpha(1-\beta)P_{2k}(t) + (1-\alpha)(1-\beta)P_{2k-1}(t) + \beta(1-\beta)P_{2k-2}(t) \quad (31)$$

$$P_{2k}(t+1) = \beta^2 P_{2k-2}(t) + \beta(1-\alpha)P_{2k-1}(t) + (1-\alpha)(1-\beta)P_{2k}(t) + \alpha(1-\alpha)P_{2k+1}(t). \quad (32)$$

From this we first compute the sublattice probabilities $P_o(t) = \sum_k P_{2k+1}(t)$ and $P_e(t) = \sum_k P_{2k}(t)$ then find the shock on the odd or even sublattice.

It is convenient to define a sublattice probability vector

$$|P(t)\rangle = \begin{pmatrix} P_o(t) \\ P_e(t) \end{pmatrix}. \quad (33)$$

Then we obtain from (31), (32)

$$|P(t+1)\rangle = \Lambda |P(t)\rangle \quad (34)$$

with the time evolution operator

$$\Lambda = \begin{pmatrix} 1 - (\alpha + \beta)(1 - \alpha) & (\alpha + \beta)(1 - \beta) \\ (\alpha + \beta)(1 - \alpha) & 1 - (\alpha + \beta)(1 - \beta) \end{pmatrix}. \quad (35)$$

The formal solution of (34) has the simple form

$$|P(t)\rangle = \Lambda^t |P(0)\rangle \quad (36)$$

where $|P(0)\rangle$ is the initial distribution of the shock position on the even or odd sublattice.

In order to obtain the long time behaviour we diagonalize Λ . The two eigenvalues λ_i are

$$\lambda_1 = 1, \quad \lambda_2 = (\alpha + \beta - 1)^2 \equiv \lambda. \quad (37)$$

Since Λ is not symmetric the left and right eigenvector are not Hermitian conjugate. Instead we find for the right eigenvectors

$$|1\rangle = \frac{1}{2 - \alpha - \beta} \begin{pmatrix} 1 - \beta \\ 1 - \alpha \end{pmatrix}, \quad |2\rangle = \frac{1}{2 - \alpha - \beta} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (38)$$

and for the left eigenvectors

$$\langle 1| = (1, 1), \quad \langle 2| = (1 - \alpha, -(1 - \beta)). \quad (39)$$

These vectors form an orthonormal basis with scalar product $\langle i|j\rangle = \delta_{i,j}$. Notice that because of probability conservation $\langle S| = \langle 1|$ is a left eigenvector of Λ with eigenvalue 1. The right eigenvector with eigenvalue 1 represents the stationary distribution, i.e. $|1\rangle = |P_*\rangle$. Now we can write

$$\Lambda^t = |P_*\rangle \langle S| + \lambda^t |2\rangle \langle 2| \quad (40)$$

and therefore

$$|P(t)\rangle = |P_*\rangle + \lambda^t \langle 2|P(0)\rangle |2\rangle. \quad (41)$$

Hence the relaxation of the sublattice distribution to stationarity is exponential with relaxation time $\tau = 1/\ln|\lambda|$. For $\lambda = 0$ the relaxation is immediate.

Next we study the mean drift of the shock. To this end we introduce the sublattice first moments $Q_o(t) = \sum_k (2k+1)P_{2k+1}(t)$ and $Q_e(t) = \sum_k 2kP_{2k}(t)$ and the first-moment vector

$$|Q(t)\rangle = \begin{pmatrix} Q_o(t) \\ Q_e(t) \end{pmatrix}. \quad (42)$$

Then we obtain from (31), (32)

$$|Q(t+1)\rangle = \Lambda|Q(t)\rangle + A|P(t)\rangle \quad (43)$$

with

$$A = \begin{pmatrix} -2\alpha^2 & (\beta - \alpha)(1 - \beta) \\ (\beta - \alpha)(1 - \alpha) & 2\beta^2 \end{pmatrix}. \quad (44)$$

Equation (43) has the structure

$$|\Phi(t+1)\rangle = \Lambda|\Phi(t)\rangle + |\Psi(t)\rangle. \quad (45)$$

This recursion has the formal solution

$$|\Phi(t)\rangle = \Lambda^t |\Phi(0)\rangle + \sum_{n=0}^{t-1} \Lambda^n |\Psi(t-1-n)\rangle. \quad (46)$$

This yields

$$|Q(t)\rangle = \Lambda^t |Q(0)\rangle + \sum_{n=0}^{t-1} \Lambda^n A \Lambda^{t-1-n} |P(0)\rangle. \quad (47)$$

In order to compute $\langle X(t) \rangle = \langle S|Q(t) \rangle$ we have to fix the initial values in this solution. We assume that at time zero the shock is at site zero. Then $|Q(0)\rangle = 0$ and

$$|P(0)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (48)$$

After some straightforward algebra this gives

$$\begin{aligned} \langle X(t) \rangle &= \langle S|A|P_*\rangle t + \frac{1 - \lambda^t}{1 - \lambda} \langle S|A|2\rangle \langle 2|P(0)\rangle \\ &= \frac{1}{2 - \alpha - \beta} \left[2(\beta - \alpha)t + (1 - \beta)(\alpha + \beta)^2 \frac{1 - \lambda^t}{1 - \lambda} \right] \end{aligned} \quad (49)$$

and we read off the drift velocity of the shock

$$v_s = \lim_{t \rightarrow \infty} \frac{\langle X(t) \rangle}{t} = \langle S|A|P_*\rangle = 2 \frac{\beta - \alpha}{2 - \alpha - \beta}. \quad (50)$$

As expected, this expression agrees with the general form of the drift velocity (15). It can be obtained directly from stationary sublattice occupation probabilities (38) and the right and left jump rates through the formula $v_s = 2(\beta P_e - \alpha P_o)$.

Finally we consider the fluctuations of the shock position. To this end we define the sublattice second-moment vector

$$|R(t)\rangle = \begin{pmatrix} R_o(t) \\ R_e(t) \end{pmatrix} \quad (51)$$

with the sublattice moments $R_o(t) = \sum_k (2k+1)^2 P_{2k+1}(t)$ and $R_e(t) = \sum_k (2k)^2 P_{2k}(t)$. The master equations (31) and (32) yield

$$|R(t+1)\rangle = \Lambda |R(t)\rangle + 2A|Q(t)\rangle + B|P(t)\rangle \quad (52)$$

with the matrix

$$B = \begin{pmatrix} 4\alpha^2 & (\alpha + \beta)(1 - \beta) \\ (\alpha + \beta)(1 - \alpha) & 4\beta^2 \end{pmatrix}. \quad (53)$$

Using (46) we find

$$\begin{aligned} |R(t)\rangle &= \Lambda^t |R(0)\rangle + 2 \sum_{n=0}^{t-1} \Lambda^n A \Lambda^{t-1-n} |Q(0)\rangle + 2 \sum_{n=0}^{t-1} \Lambda^n A \sum_{k=n}^{t-2} \Lambda^{k-n} A \Lambda^{t-2-k} |P(0)\rangle \\ &\quad + \sum_{n=0}^{t-1} \Lambda^n B \Lambda^{t-1-n} |P(0)\rangle. \end{aligned} \quad (54)$$

Now we observe that $|R(0)\rangle = 0$. Therefore the first line in this equation does not contribute. Using the expansion (40) we obtain

$$\begin{aligned} \langle X^2(t) \rangle &= 2 \sum_{n=0}^{t-1} \sum_{k=n}^{t-2} [\langle S|A|P_* \rangle^2 + \lambda^{k-n} \langle S|A|2 \rangle \langle 2|A|P_* \rangle + \lambda^{t-2-k} \langle S|A|P_* \rangle \langle S|A|2 \rangle \langle 2|P(0) \rangle \\ &\quad + \lambda^{t-2-n} \langle S|A|2 \rangle^2 \langle 2|P(0) \rangle] + \sum_{n=0}^{t-1} [\langle S|A|P_* \rangle + \lambda^{t-1-n} \langle S|B|2 \rangle \langle 2|P(0) \rangle]. \end{aligned} \quad (55)$$

The scalar products are easy to compute using the explicit expressions for the eigenvectors of T and matrices A, B given above. Putting everything together we finally arrive after some more straightforward algebra at

$$D = \lim_{t \rightarrow \infty} \frac{\langle X^2(t) \rangle - \langle X(t) \rangle^2}{2t} = 4 \frac{(\alpha + \beta)(1 - \alpha)(1 - \beta)}{(2 - \alpha - \beta)^3}. \quad (56)$$

Fluctuations are large for ‘small’ shocks where both ρ_1 and ρ_2 differ only slightly from $1/2$ and they are small if only one of two densities is close to $1/2$. If one density is exactly $1/2$ ($\alpha = 1$ or $\beta = 1$) the shock moves ballistically. Along the line $\beta = 1 - \alpha$ where the eigenvalue λ vanishes the diffusion coefficient takes the simple form $D = 4\alpha(1 - \alpha)$.

3.3. Shock motion as a random walk with internal degree of freedom

The sublattice dynamics of the shock position can be interpreted in a different way by assigning a binary internal degree of freedom $f = \pm$ to the random walker. This degree of freedom denotes the present direction of motion. The dynamics in one time step are as follows. If the walker is in state $+$ it can move to the right with probability β or reverse direction (without moving) and go to state $-$ with probability $1 - \beta$. On the other hand, if the walker is in state $-$ it can move to the left with probability α or reverse direction (without moving) and go to state $+$ with probability $1 - \alpha$. So after one time step the following transitions may occur:

$$(k, +) \rightarrow \begin{cases} (k, -) & \text{with probability } 1 - \beta \\ (k + 1, +) & \text{with probability } \beta \end{cases} \quad (57)$$

$$(k, -) \rightarrow \begin{cases} (k, +) & \text{with probability } 1 - \alpha \\ (k - 1, -) & \text{with probability } \alpha. \end{cases} \quad (58)$$

Iterating yields the evolution after two steps:

$$(k, +) \rightarrow \begin{cases} (k - 1, -) & \text{with probability } \alpha(1 - \beta) \\ (k, +) & \text{with probability } (1 - \alpha)(1 - \beta) \\ (k + 1, -) & \text{with probability } \beta(1 - \beta) \\ (k + 2, +) & \text{with probability } \beta^2 \end{cases} \quad (59)$$

$$(k, -) \rightarrow \begin{cases} (k - 2, -) & \text{with probability } \alpha^2 \\ (k - 1, +) & \text{with probability } \alpha(1 - \alpha) \\ (k, -) & \text{with probability } (1 - \alpha)(1 - \beta) \\ (k + 1, +) & \text{with probability } \beta(1 - \alpha). \end{cases} \quad (60)$$

Notice that after two steps the internal state $\pm$ does not leave its original sublattice. For example, if at time zero the walker is in a positive state on the even sublattice, then at all even times it will be positive on the even sublattice and negative on the odd sublattice. Therefore two time steps of this random walk with speed flip are equivalent to a single time step in the random walk with sublattice update.

4. Open boundaries

The theory of boundary-induced phase transitions postulates that for stochastic interacting particle systems the random motion of a shock causes a discontinuous non-equilibrium phase transition from a low-density phase to a high-density phase [23]. With the results of the section 3 we have proved the validity of this heuristic argument for the slCA184 with deterministic bulk dynamics. Moreover, it turns out that we can explicitly compute relaxation times. To this end we have to specify the dynamics of the second-class particle at the open boundaries of the system.

4.1. Open boundaries and second-class particle

It is helpful to think of the injection and removal of particles as input and output from particle reservoirs. Indeed, we can represent these reservoirs as sites $0, L + 1$ on the

integer lattice [16] where in the presence of a single second-class particle in the system each reservoir site can be in two states, the reservoir state (denoted R for right or left boundary respectively) or the second-class particle state (denoted F). In terms of these states the update rules of the boundary sites are:

left boundary $k = 1$ with reservoir states R, F at $k = 0$:

$$\begin{aligned} R0 &\rightarrow RA && \text{with probability } \alpha \\ RB &\rightarrow BA && \text{with probability } \alpha \\ F0 &\rightarrow RB && \text{with probability } 1. \end{aligned} \quad (61)$$

The configurations $R0$ and RB remain unchanged with probability $1 - \alpha$.

Right boundary $k = L$ with reservoir states R, F at $k = L + 1$:

$$\begin{aligned} AR &\rightarrow 0R && \text{with probability } \beta \\ BR &\rightarrow 0F && \text{with probability } \beta \\ AF &\rightarrow BR && \text{with probability } 1. \end{aligned} \quad (62)$$

The configurations AR and BR remain unchanged with probability $1 - \beta$.

Correspondingly we have to redefine the shock measures (22), (23) to include the boundary state. We represent the reservoir state by the basis vectors

$$|R\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |F\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (63)$$

and also define measures for the bulk sites $1, \dots, L$

$$|\mu_{\text{low}}\rangle = |\alpha\rangle \otimes |0\rangle \otimes |\alpha\rangle \otimes |0\rangle \otimes \dots \otimes |\alpha\rangle \otimes |0\rangle \quad (64)$$

$$|\mu_{\text{high}}\rangle = |\gamma\rangle \otimes |A\rangle \otimes |\gamma\rangle \otimes |A\rangle \otimes \dots \otimes |\gamma\rangle \otimes |A\rangle \quad (65)$$

where as above $\gamma = 1 - \beta$ and no second-class particles are present. With these definitions we define as new shock measures for the sites $0, \dots, L + 1$

$$|\tilde{\mu}_{L+1}\rangle = |R\rangle \otimes |\mu_{\text{low}}\rangle \otimes |F\rangle \quad (66)$$

$$|\tilde{\mu}_{2k+1}\rangle = |R\rangle \otimes |\mu_{2k+1}\rangle \otimes |R\rangle \quad (67)$$

$$|\tilde{\mu}_{2k}\rangle = |R\rangle \otimes |\mu_{2k}\rangle \otimes |R\rangle \quad (68)$$

$$|\tilde{\mu}_0\rangle = |F\rangle \otimes |\mu_{\text{high}}\rangle \otimes |R\rangle. \quad (69)$$

One may think of the state F as marking the microscopic shock position in a reservoir site.

Applying the update rules we recover equations analogous to (27) and (28) for the bulk sites with $k = 2, \dots, L/2 - 1$. In addition we obtain for the boundaries

$$T|\tilde{\mu}_{L+1}\rangle = \alpha^2|\tilde{\mu}_{L-1}\rangle + \alpha(1 - \alpha)|\tilde{\mu}_L\rangle + (1 - \alpha)|\tilde{\mu}_{L+1}\rangle \quad (70)$$

$$T|\tilde{\mu}_L\rangle = \alpha(1 - \beta)|\tilde{\mu}_{L-1}\rangle + (1 - \alpha)(1 - \beta)|\tilde{\mu}_L\rangle + \beta|\tilde{\mu}_{L+1}\rangle \quad (71)$$

$$T|\tilde{\mu}_1\rangle = \alpha|\tilde{\mu}_0\rangle + (1 - \alpha)(1 - \beta)|\tilde{\mu}_1\rangle + \beta(1 - \alpha)|\tilde{\mu}_2\rangle \quad (72)$$

$$T|\tilde{\mu}_0\rangle = (1 - \beta)|\tilde{\mu}_0\rangle + \beta(1 - \beta)|\tilde{\mu}_1\rangle + \beta^2|\tilde{\mu}_2\rangle. \quad (73)$$

Thus the evolution of the shock measures is closed under the action of slCA 184 and corresponds to a sublattice random walk as defined above, but with reflecting boundary conditions where jumps outside the integer interval $0, \dots, L+1$ are suppressed. Representing the shock position by a probability distribution $P_k(t)$ we obtain a master equation similar to (31) and (32) for $k = 1, \dots, L/2$, augmented by the boundary equations

$$P_{L+1}(t+1) = (1-\alpha)P_{L+1}(t) + \beta P_L(t) \quad (74)$$

$$P_0(t+1) = (1-\beta)P_0(t) + \alpha P_1(t). \quad (75)$$

4.2. Relaxation

First we study the stationary distribution by making an ansatz $P_{2k}^* = y^k/Z$ and $P_{2k+1}^* = A^*y^{2k+1}/Z$. The constant A^* accounts for the possibility of a sublattice structure and Z ensures normalization of the stationary distribution. This ansatz satisfies the master equation with $y = \beta/\alpha$ and $A^* = 1$. Normalization requires $Z = (1-y^{L+2})/(1-y)$. We point out a slight difference to the work [40] where the stationary distribution of slCA184 is studied using a family of shock measures without second-class particles. For that definition one has a geometric distribution of shock positions with the same parameter $y = \beta/\alpha$, but with sublattice anisotropy $A^* = 1 - \alpha - \beta$ [40].

For $\beta > \alpha$ the shock position is typically close to the right boundary with a localization length $1/\ln(\beta/\alpha)$ and exponentially decaying density profile away from the right boundary to the bulk value $\rho_1 = \alpha/2 < 1/2$. This corresponds to a low-density phase of the particle system. Conversely $\beta < \alpha$ corresponds to the high-density phase with bulk density $\rho_1 = 1 - \beta/2 > 1/2$. At the phase transition line $\beta = \alpha$ the shock position is uniformly distributed, corresponding to a linearly increasing average density profile. Hence the stationary phase of slCA 184 with second-class particle is identical to that of the original slCA184 without second-class particle [25] and to that of CA184 without second-class particle [47, 48].

In order to compute relaxation times to stationarity one has to solve the eigenvalue problem for the full master equation (31)–(75). For the solution we first ignore the boundary conditions and make the preliminary ansatz $P_k(p, t) = \Lambda^t(p)F_k(p)$ with the eigenfunction

$$F_{2k-1}(p) = A(p)y^{2k-1}e^{ip(2k-1)} \quad (76)$$

$$F_{2k}(p) = y^{2k}e^{2ipk}. \quad (77)$$

Here p is a pseudomomentum, $A(p)$ is an amplitude to be fixed by the sublattice structure of the bulk master equation and $\Lambda(p)$ is the eigenvalue corresponding to p . Inserting this ansatz into the bulk master equation (31) and (32) yields a quadratic equation for $A(p)$ with the solutions

$$A^\pm(p) = \frac{1}{2(1-\alpha)} \left[\beta e^{ip} - \alpha e^{-ip} \pm \sqrt{(\beta e^{ip} + \alpha e^{-ip})^2 + 4(1-\alpha-\beta)} \right]. \quad (78)$$

With this one obtains corresponding eigenvalues

$$\Lambda^\pm(p) = x + 2y^2 \pm 2y\sqrt{y^2 + x} \quad (79)$$

where

$$x = 1 - \alpha - \beta, \quad y = (\beta e^{ip} + \alpha e^{-ip})/2. \quad (80)$$

Notice the symmetry relation $\Lambda^\pm(p) = \Lambda^\pm(i \ln(\beta/\alpha) - p)$. Hence the most general eigenfunction with eigenvalue $\Lambda^\pm(p)$ has the form

$$G_k(p) = F_k(p) + R(p)F_k(i \ln(\beta/\alpha) - p) \quad (81)$$

with the boundary conditions

$$\beta^2 F_{-2} + \beta(1 - \alpha)F_{-1} - \alpha(1 - \beta)F_0 - \alpha^2 F_1 = 0 \quad (82)$$

$$\alpha^2 F_{L+3} + \alpha(1 - \beta)F_{L+2} - \beta(1 - \alpha)F_{L+1} - \beta^2 F_L = 0. \quad (83)$$

which are obtained from (74) to (75) by equating these relations to the bulk relations (31) and (32) for $k = 0$ and $k = L + 1$ respectively. The boundary conditions determine the reflection amplitude $R(p)$ and give rise to an eigenvalue equation for the pseudomomenta p . Generically this is a transcendental equation for which one cannot write solutions in closed form. However, it turns out that along the curve $\beta = 1 - \alpha$ the algebra simplifies very considerably and closed expressions for the solutions can be obtained. This curve runs across the phase diagram and therefore captures all the essential features of the two phases and the phase transition line. Therefore in what follows we restrict ourselves to this case. Notice that we exclude the trivial limiting cases $\alpha = 0$ and 1 where the shock moves deterministically backward on the odd sublattice or forward on the even sublattice respectively until it hits the boundary where it remains fixed for all times.

For $\beta = 1 - \alpha$ one has

$$A^+(p) = e^{ip}, \quad A^-(p) = -\frac{\alpha}{1 - \alpha}e^{-ip} \quad (84)$$

and

$$\Lambda^+(p) = ((1 - \alpha)e^{ip} + \alpha e^{-ip})^2, \quad \Lambda^-(p) = 0. \quad (85)$$

and the eigenfunctions have the simple form

$$G_{2k}(p) = \left(\frac{1 - \alpha}{\alpha}\right)^{2k} e^{2ipk} + R(p)e^{-2ipk} \quad (86)$$

$$G_{2k-1}(p) = \frac{\alpha}{1 - \alpha}G_{2k}(p). \quad (87)$$

The left boundary condition (82) yields

$$R(p) = \frac{(1 - \alpha)e^{2ip} - (1 - 2\alpha) - \alpha e^{-2ip}}{(1 - \alpha)^3 e^{2ip} + \alpha(1 - \alpha)(1 - 2\alpha) - \alpha^3 e^{-2ip}}. \quad (88)$$

With this result the right boundary condition (83) factorizes into the form

$$\left[\left(\frac{1 - \alpha}{\alpha}\right)^{L+2} e^{2ip(L+2)} - 1 \right] (1 - e^{2ip}) ((1 - \alpha) + \alpha e^{-2ip}) = 0. \quad (89)$$

For non-vanishing eigenvalues $\Lambda_n \equiv \Lambda(p_n)$ this has the solution $p = 0$ which corresponds to the stationary distribution with eigenvalue $\Lambda = 1$ and the relaxation solutions with

$$p_n = \frac{1}{2i} \ln \left(\frac{\alpha}{1-\alpha} \right) + \frac{n\pi}{L+2}, \quad n = 0, 1, \dots, L/2. \quad (90)$$

Therefore

$$\Lambda_n = D \cos^2 \left(\frac{n\pi}{L+2} \right) \quad (91)$$

where $D = 4\alpha(1-\alpha)$ is the shock diffusion coefficient.

The relaxation spectrum ϵ_n with the inverse of the relaxation times $\tau_n = 1/\epsilon_n$ is defined by the expression $\Lambda_n^t = \exp(-\epsilon_n t)$. This yields the longest relaxation time $\tau^* = 1/\ln D$. At the phase transition point $\alpha = 1/2$ the relaxation is diffusive. For large system size L one has asymptotically

$$\tau_n = \frac{L^2}{\pi^2 n^2} \quad (92)$$

and in particular the longest relaxation time $\tau^* = L^2/\pi^2$.

5. Conclusions

In summary, we have studied the large-scale behaviour of a CA that corresponds to the deterministic limit of the TASEP with sublattice update and we have investigated the microscopic properties of shock solutions to the hydrodynamic equation (16) that corresponds to these dynamics. An essential microscopic feature that produces shocks on the macroscale seems to be a sufficiently strong bulk driving force. Purely boundary-driven or weakly irreversible particle hopping models do not exhibit traffic jams, which is also in agreement with experimental results, see for example [41]–[43] for some well-established applications of such models to experiments on soft matter systems. On the other hand, we conclude from our present study that noise in the dynamics does not seem to be necessary to generate shocks. Indeed, the absence of noise does not even necessarily alter the internal microscopic structure of a shock.

However, the time evolution inherits non-trivial randomness from the initial distribution of particles (in an infinite system) or from random injection/removal of particles at the boundaries of a finite system. The main results of our analysis are as follows.

- (1) The evolution of the coarse-grained density exhibits shocks on the macroscopic scale, travelling with average velocity (15). For initial downward steps with $\rho_1 > 1/2 > \rho_2$ a double step structure with an intermediate density $1/2$ develops. This structure is the analogue of a rarefaction wave. On the microscopic scale this constant profile is realized by an alternating particle–vacancy configuration.
- (2) We have defined a microscopic marker particle using the second-class particle technique. Seen from the position of this particle, which we define as the microscopic shock position, a product measure with alternating densities as in the stationary state of a translation-invariant periodic system is also stationary inside the two branches of the shock, similar to the family of shock measures without second-class particles that

was introduced in [40]. The second-class particle performs a random walk with speed flip. We have computed analytically the shock velocity and diffusion coefficient of the shock. Our results are exact and valid for all densities ρ_1, ρ_2 of the two branches of the shock. This is in contrast to the stochastic TASEP with sublattice update where analogous results are valid only for a one-dimensional parameter manifold of shock densities [44, 45].

- (3) For a finite system with open boundaries we have found that the long time dynamics are given by a microscopic shock (traffic jam) that performs a biased random walk with reflecting boundaries. We have computed explicitly the relaxation times along a specific, but generic curve in the phase diagram. Away from the phase transition point the longest relaxation time is finite even in the thermodynamic limit and given by the shock diffusion coefficient. The stationary density profile has a boundary layer whose structure is solely determined by microscopic fluctuations of the shock which is pinned to the boundary on the macroscopic scale. At the phase transition point the shock performs an unbiased random walk and the longest relaxation time diverges quadratically with system size. Therefore the system is dynamically critical with dynamical exponent $z = 2$. On the macroscopic scale this corresponds to a step function profile where the shock is located at an arbitrary position.

The microscopic sharpness of the shock, which is implicit in our construction, is useful for applying hydrodynamic arguments to a finite lattice, as it allows for a good approximate description of dynamics on the lattice scale in terms of macroscopic arguments involving shocks [46]. The stationary phase diagram is similar to that of CA184 [47, 48], as predicted by the general theory of boundary-induced phase transitions. It would be interesting to investigate the boundary layers in CA 184 in more detail in order to gain a better understanding of the interplay of the fluctuating shock position and boundary correlations which in general determine the microscopic structure of the boundary layer.

We finish with a remark of a general nature on the microscopic dynamics of the shock. Quasi-one-dimensional random motion with stochastic speed flips occurs in various biological systems, in particular in cargo transport by molecular motors along microtubules in cells. To explain the alternating direction of motion, some authors postulate a coordination complex that prevents one group of motors from performing during some period of time. Some external stimulus is assumed to determine the activity of the coordination complex. A different mechanism that has been proposed in recent years is a tug-of-war: two intrinsically oppositely moving motor species attach to the cargo at the same time and try to pull the cargo in their intrinsic direction of motion. Due to fluctuations, sometimes one group of motors ‘wins’ over the other. Quantitative predictions from a tug-of-war model have been checked against experimental data from lipid droplet transport in *Drosophila* embryos [49]. Good agreement with experimental data suggests that indeed the collective tug-of-war mechanism is responsible for the observed reversal of motion rather than the action of some external coordination complex. From a statistical physics perspective this observation is interesting in so far as it demonstrates that a tug-of-war is a generic collective mechanism for motion with stochastic speed change. This system is only one example of a biological process with stochastic speed change. Another example is the run-and-tumble dynamics of certain

bacteria, see [50] for recent work on this problem. It is therefore interesting on general grounds to understand which collective processes can lead to the motion of a single particle with stochastic speed change. Our model provides such a mechanism, where the speed changes are triggered by the arrival of clusters of first-class particles from the right or vacancies from the left.

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