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# Microscopic structure of travelling wave solutions in a class of stochastic interacting particle systems

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**Abstract.** We obtain exact travelling wave solutions for three families of stochastic one-dimensional non-equilibrium lattice models with open boundaries. These solutions describe the diffusive motion and microscopic structure of (i) shocks in the partially asymmetric exclusion process with open boundaries, (ii) a lattice Fisher wave in a reaction–diffusion system, and (iii) a domain wall in non-equilibrium Glauber–Kawasaki dynamics with magnetization current. For each of these systems we define a microscopic shock position and calculate the exact hopping rates of the travelling wave in terms of the transition rates of the microscopic model. In the steady state a reversal of the bias of the travelling wave marks a first-order non-equilibrium phase transition, analogous to the Zel'dovich theory of kinetics of first-order transitions. The stationary distributions of the exclusion process with $n$ shocks can be described in terms of $n$-dimensional representations of matrix product states.


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**Contents**



## 1. Introduction

Systems of diffusing and reacting particles are usually described on the macroscopic level by hydrodynamic equations for coarse-grained quantities like the particle density which represent the order parameter specifying the macroscopic state of the system [1]. Paradigmatic examples for these equations are the Burgers equation for driven diffusive systems with particle conservation [2] or the Fisher equation for reactive systems without conservation law [3, 4]. These equations are, in general, non-linear and exhibit shocks in some cases. This means that the solution of the macroscopic equations may develop a discontinuity even if the initial particle density is smooth. In order to understand the emergence of such behaviour from the microscopic laws that govern the stochastic motion and interaction of particles it is necessary to *derive* the macroscopic equations from the microscopic dynamics rather than postulating them on phenomenological grounds. To solve this problem it is evident that detailed insight in the microscopic structure of non-equilibrium systems exhibiting macroscopic discontinuities must be obtained.

A considerable body of results of this nature has been obtained for specific one-dimensional lattice models defined on the integer lattice $\mathbb{Z}$ [5]–[7], the best-studied example being the asymmetric simple exclusion process (ASEP) [8, 9]. In this basic model for a driven diffusive system, each site $k$ is either empty ($n_k = 0$) or occupied by at most one particle ($n_k = 1$). A particle on site $k$ hops randomly to the site $k+1$ with rate $D_{\mathrm{r}}$ and to the site $k-1$ with rate $D_{\mathrm{l}}$, but only if the target site is empty. Otherwise the attempted move is rejected. The jumps occur independently in continuous time with an exponential waiting time distribution. In the hydrodynamic limit the system is described by the Burgers equation which exhibits shocks. Such a shock discontinuity may be viewed as the interface between stationary domains of different densities. Relaxing the requirement of particle number conservation leads to a class of systems which are generically called reaction–diffusion processes, but which by a variety of mappings also serve as toy models for non-conservative spin-flip dynamics (in the context of magnetic systems), epidemic spreading, growth processes and transport phenomena in biological and ecological systems and elsewhere [9, 10].

Most of the results for the dynamical behaviour have been obtained for infinite particle systems. In many of the physical applications, however, one has to study finite systems with open boundaries where particles are injected and extracted. This is crucial to take into account as—in the absence of equilibrium conditions—the boundary conditions determine the bulk behaviour of driven systems, even to the extent that boundary induced phase transitions between bulk states of different densities occur [11]–[13]. Qualitatively, the strong effect of boundary conditions on the bulk can be attributed to the presence of steady-state currents which carry boundary effects into the bulk of the system. Quantitatively, exact results for the steady state of the ASEP have helped to show that part of the non-equilibrium phase diagram of driven diffusive systems with open boundaries, namely phase transitions of first order, can be understood from the diffusive motion of shocks [14, 15], analogous to the Zel'dovich theory of equilibrium kinetics of first-order transitions. As in equilibrium, the non-equilibrium theory of boundary-induced phase transitions requires the existence of shocks which are microscopically sharp.

In a series of recent papers [16]–[19] these considerations, originally formulated for conservative dynamics, have been extended to non-conservative reaction–diffusion systems. Moreover, there are exact results about shocks in reaction–diffusion systems with branching and coalescence [20]–[25] (here shocks are known as Fisher waves on the macroscopic scale) and in spin-flip systems where shocks correspond to domain walls [26]. However, no exact results have been reported so far for non-stationary travelling waves in open systems. Here we wish

(i) to establish a complete picture about exact travelling wave solutions for the specific family of systems to which these processes belong (namely single-species exclusion processes with two-body nearest-neighbour interaction and no internal degrees of freedom) and
(ii) to study the dynamics and microscopic structure of these travelling shocks in systems with *open boundaries*.

Since many of the powerful techniques used for treating the ASEP do not apply to non-conservative systems, we propose a general approach that can be applied to any lattice model: we take as initial distribution a shock distribution with given microscopic properties and determine the class of models for which the shock distribution evolves into a linear combination of similar distributions with different shock positions. In this paper we identify three families of processes with this property.

The paper is organized as follows: in the following section we define the class of models that we consider and we also define shock measures for these systems. In section 3 we determine the families of models with travelling wave solutions on the finite lattice. This is followed by some new results for the ASEP with open boundaries in section 4. In section 5 we summarize our results and draw some conclusions.

## 2. Reaction–diffusion systems and shock measures

### 2.1. Stochastic single-species models

We consider Markovian interacting particle systems of a single species of particles without internal degrees of freedom which have hard-core two-body interactions with their nearest-neighbour sites. We describe hard-core interaction due to excluded volume in terms of an exclusion process where each lattice site may be occupied by at most one particle. This class of models may therefore be described by a set of occupation numbers $\underline{n} = \{n_1, \ldots, n_L\}$ where $n_k = 0, 1$ is the number of particles on site $k$ on a lattice of $L$ sites. There is a one-to-one correspondence to classical spin systems where the occupation number $n_k = 0$ represents spin-up while $n_k = 1$ represents spin-down.

The stochastic dynamics are defined in terms of transition rates (transition probabilities per infinitesimal time unit). The process is fully defined by the 12 rates $w_{ij}$ for changes of the configuration of a pair of neighbouring sites $k$ and $k+1$ [27]:

$$w_{ij} : (n_k n_{k+1}) \to (n'_k n'_{k+1}), \tag{1}$$

where $i = 1, 2, 3, 4$ is the decimal value plus one of the target configuration $(n'_k n'_{k+1})$ read as a two-digit binary number and $j$ is the respective value of the initial configuration $(n_k n_{k+1})$, as shown below.

| | |
|---|---|
| Diffusion to the left and right ($01 \rightleftharpoons 10$) | $w_{32}, w_{23}$ |
| Coalescence to the left and right ($11 \to 10, 01$) | $w_{34}, w_{24}$ |
| Branching to the left and right ($10, 01 \to 11$) | $w_{43}, w_{42}$ |
| Death to the left and right ($10, 01 \to 00$) | $w_{13}, w_{12}$ |
| Birth to the left and right ($00 \to 10, 01$) | $w_{31}, w_{21}$ |
| Pair annihilation and creation ($11 \rightleftharpoons 00$) | $w_{14}, w_{41}$. |

From time to time we also use the more intuitive symbols $D_{\mathrm{r}} = w_{23}$, $D_{\mathrm{l}} = w_{32}$ for the hopping rates. Notice that combinations of individual processes may describe other physically meaningful processes. For example, coalescence and death with equal rates is equivalent to single-site radioactive decay ($1 \to 0$) with that rate. The inverse of the rate is the mean life time of a particle. For injection and extraction of particles at the boundaries we introduce the rates

| | |
|---|---|
| Injection and extraction at the left boundary ($0 \rightleftharpoons 1$) | $\alpha, \gamma$ |
| Injection and extraction at the right boundary ($0 \rightleftharpoons 1$) | $\delta, \beta$. |

The time evolution is defined by a continuous-time master equation for the distribution $P(n_1, \ldots, n_L; t)$ which we write in terms of the quantum Hamiltonian formalism [9]. The distribution is mapped to a probability vector $|P(t)\rangle$ which contains as components the probabilities $P(n_1, \ldots, n_L; t)$. The time evolution is generated by the stochastic Hamiltonian $H$ whose matrix elements are the transition rates between configurations. The Markovian time evolution can then conveniently be cast in the form of an imaginary time Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|P(t)\rangle - H|P(t)\rangle \tag{2}$$

with the formal solution

$$|P(t)\rangle = \mathrm{e}^{-Ht}|P(0)\rangle. \tag{3}$$

The quantum Hamiltonian $H$ for the family of processes defined above has the structure

$$H = \sum_{k=1}^{L-1} h_k + b_1 + b_L. \tag{4}$$

Here

$$h_k = -\begin{pmatrix} \cdot & w_{12} & w_{13} & w_{14} \\ w_{21} & \cdot & w_{23} & w_{24} \\ w_{31} & w_{32} & \cdot & w_{34} \\ w_{41} & w_{42} & w_{43} & \cdot \end{pmatrix}_{k,k+1} \tag{5}$$

is the local transition matrix acting non-trivially on sites $k, k+1$. The diagonal elements are the negative sum of the transitions rates in the respective column, as required by conservation of probability. The boundary matrices

$$b_1 = -\begin{pmatrix} -\alpha & \gamma \\ \alpha & -\gamma \end{pmatrix}_1, \qquad b_L = -\begin{pmatrix} -\delta & \beta \\ \delta & -\beta \end{pmatrix}_L \tag{6}$$

generate the boundary processes.

The invariant measures $|P^*\rangle$ of the process, i.e., the stationary probability distributions, satisfy the eigenvalue equation

$$H|P^*\rangle = 0. \tag{7}$$

We stress that the analogy to quantum mechanics is a formal one; for details see [9].

The equations of motion for the expected local particle density take the form [27]

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle n_x(t)\rangle &= B_1\langle n_{x-1}(t)\rangle + B_2\langle n_{x+1}(t)\rangle - (C_1 + C_2)\langle n_x(t)\rangle \\ &\quad + D_1\langle n_{x-1}(t)n_x(t)\rangle + D_2\langle n_x(t)n_{x+1}(t)\rangle + A_1 + A_2 \end{aligned} \tag{8}$$

with

$$\begin{array}{ll} A_1 = w_{21} + w_{41} & B_1 = w_{23} + w_{43} - w_{21} - w_{41} \\ C_1 = w_{12} + w_{32} + w_{21} + w_{41} & D_1 = C_1 - w_{23} - w_{43} - w_{14} - w_{34} \\ A_2 = w_{31} + w_{41} & B_2 = w_{32} + w_{42} - w_{31} - w_{41} \\ C_2 = w_{13} + w_{23} + w_{31} + w_{41} & D_2 = C_2 - w_{32} - w_{42} - w_{14} - w_{24}. \end{array} \tag{9}$$

In analysing these equations the question arises of how to treat the non-linearity in the lattice equation, i.e. the two-point correlator $D_1\langle n_{x-1}(t)n_x(t)\rangle + D_2\langle n_x(t)n_{x+1}(t)\rangle$. Calculating its time-derivative leads to a coupling to three-point correlation functions and eventually to a hierarchy of equations which is just as untractable as the master equation itself. Only for some families of models does the system of equations decouple and exact results are obtained [20], [27]–[30]. Therefore here we do not follow this traditional approach but rather investigate the time evolution of the measures.

### 2.2. *Product measures and shock measures*

The stationary distribution of the family of processes defined above depends on all the transition rates and is not known in general. On some parameter manifolds, however, the stationary distributions are simple Bernoulli product measures

$$P^*(\underline{n}) = \prod_{j=1}^{L}((1-\rho)\delta_{n_j,0} + \rho\delta_{n_j,1}) \tag{10}$$

where the probability of finding a particle at each site $k$ is $\rho$ and independent of the occupation of other lattice sites, i.e. where there are no correlations. It is easy to see that $P^*$ depends only on the total number $N = \sum_k n_k$ of particles in the configuration $\underline{n}$, and one has $P^*(\underline{n}) = (1-\rho)^{L-N}\rho^N$.

In the quantum Hamiltonian formulation this distribution is represented by a tensor state

$$|P^*\rangle = \begin{pmatrix} 1-\rho \\ \rho \end{pmatrix}^{\otimes L} \equiv |\rho\rangle. \tag{11}$$

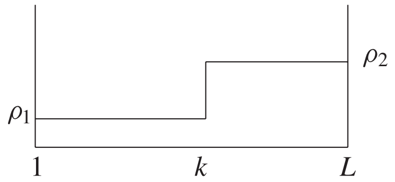


**Figure 1.** Density profile of a Bernoulli shock measure.

The family of processes for which this is an invariant measure can be determined easily from (7). One first determines the manifold of bulk rates $w_{ij}$ such that

$$h_k|\rho\rangle = A(n_{k+1} - n_k)|\rho\rangle \tag{12}$$

with an arbitrary constant $A$. This yields three equations for the 12 bulk parameters. The solutions define a manifold of processes with uncorrelated stationary distributions, provided the system has periodic boundary conditions. In order to satisfy (7) for systems with open boundaries one determines the boundary parameters by the relations

$$b_1|\rho\rangle = An_1|\rho\rangle, \qquad b_L|\rho\rangle = -An_L|\rho\rangle. \tag{13}$$

For each boundary this is one equation for two rates. Notice that these relations contain the stationary particle density $\rho$ as free parameter.

Bernoulli shock measures are product measures with a jump in the density at some site $m$ (figure 1). They are represented by a tensor state

$$|k\rangle_{\rho_1,\rho_2} = \begin{pmatrix} 1-\rho_1 \\ \rho_1 \end{pmatrix}^{\otimes k} \otimes \begin{pmatrix} 1-\rho_2 \\ \rho_2 \end{pmatrix}^{\otimes L-k}. \tag{14}$$

There are no correlations, but the density in the left domain of sites $1, \ldots, k$ is $\rho_1$ and then jumps to $\rho_2$ in the right domain $k+1, \ldots, L$ of the system. Since there are no correlations one may regard the lattice unit as the intrinsic shock width. Hence shocks which are described by a such a distribution are microscopically sharp and have a very simple internal structure, characterized by the absence of any correlation between particle positions. There is no process of the form (4) for which a shock distribution with a shock at some given site $k$ is stationary. However, as shown in the next section, linear combinations of shock measures may be stationary distributions. Notice that a shock at position $m = 0$ corresponds to a Bernoulli measure with density $\rho_2$ while a shock at position $k = L$ corresponds to a Bernoulli measure with density $\rho_1$.

## 3. Shocks as stable collective excitations

A linear combination of shock measures is a stationary measure if a given shock measure evolves into a linear combination of shock measures after time $t$, i.e. where $|P(t)\rangle_{m,\rho_1,\rho_2} \equiv \exp(-Ht)|m\rangle_{\rho_1,\rho_2}$ has the form

$$|P(t)\rangle_{m,\rho_1,\rho_2} = \sum_{k=0}^{L} p(m,k;t)|k\rangle_{\rho_1,\rho_2}. \tag{15}$$

The physical interpretation of this property is that a shock retains its internal structure at all times, only the position of the shock is shifted by a random amount. The probability of moving from the initial shock position $m$ to site $k$ after time $t$ is the quantity $p(m, k; t)$. Hence we shall refer to measures of the form (15) as diffusive shock measures. The random walk nature of such a shock gives rise to the interpretation as a collective single-particle excitation. This can be made more precise by the implications of (15). The evolution into a linear combination of shock measures implies, for an infinitesimal step (which is generated by $H$), the evolution equation

$$-H|m\rangle_{\rho_1,\rho_2} = d_1|m-1\rangle_{\rho_1,\rho_2} + d_2|m+1\rangle_{\rho_1,\rho_2} - (d_1+d_2)|m\rangle_{\rho_1,\rho_2} \tag{16}$$

which is the evolution equation for a biased single-particle random walk with hopping rate $d_2$ to the right and hopping rate $d_1$ to the left. Hence we have to determine processes such that (16) is satisfied. The family of shock distributions defined by the densities $\rho_1$, $\rho_2$ forms an invariant sector $\mathcal{U}$ under the time evolution of the system. Notice that (16) implies the existence of at least two stationary product solutions in a periodic system. These stationary states have densities $\rho_1$, $\rho_2$, respectively. The boundary rates have to be chosen such that at the left boundary $\rho_1$ is stationary, while at the right boundary $\rho_2$ is stationary.

Solving (16) leads to three classes of reaction–diffusion models with an invariant sector $\mathcal{U}$ which are described below.

### *3.1. Asymmetric simple exclusion process (ASEP)*

The simplest process which satisfies (16) is the ASEP with hopping to the left and right (without loss of generality we assume a bias to the right) and injection and extraction at both boundaries. Hence the non-vanishing rates

$$w_{32}, \quad w_{23}, \quad \gamma, \quad \alpha, \quad \beta, \quad \delta. \tag{17}$$

These rates, together with the densities $\rho_1$ and $\rho_2$, satisfy the following conditions:

$$w_{23} = \frac{(1-\rho_1)\rho_2}{\rho_1(1-\rho_2)} w_{32} \tag{18}$$

$$\alpha(1-\rho_1) - \gamma\rho_1 = (w_{23} - w_{32})\rho_1(1-\rho_1) \tag{19}$$

$$\beta\rho_2 - \delta(1-\rho_2) = (w_{23} - w_{32})\rho_2(1-\rho_2). \tag{20}$$

Both densities have to fulfil the conditions $0 < \rho_1 < \rho_2 < 1$ in this case. Condition (18) was obtained for the infinite system in [31] using symmetry properties of the quantum Hamiltonian (see next section). In the bulk of the lattice the shock position moves like a biased lattice random walk with hopping rates

$$d_i = (D_\mathrm{r} - D_\mathrm{l}) \frac{\rho_i(1-\rho_i)}{\rho_2 - \rho_1} \tag{21}$$

to the left ($i = 1$) and right ($i = 2$), respectively. This leads to the well-known exact expressions for the shock velocity $v_\mathrm{s} = d_2 - d_1$ and shock diffusion coefficient $D_\mathrm{s} = (d_2 + d_1)/2$ [5, 32] as long as the shock is far from the boundaries.

The new results are conditions (19), (20) which imply that at the boundaries the shock is reflected. According to the properties of a biased random walk on a finite lattice with reflecting boundaries and bulk rates (21), its stationary position after equilibration is geometrically distributed, i.e., the probability of finding the shock at site $k$ on the lattice is of the form

$$p^*(k) \propto \left(\frac{d_2}{d_1}\right)^k. \tag{22}$$

Depending on the bias of the shock, the steady state of the system is in the low-density subphase $A_I$ (for $d_2 > d_1$), in the high-density subphase $B_I$ (for $d_1 > d_2$) or on the first-order coexistence line (for $d_1 = d_2$) [12, 33]. From (22) we read off the exact inverse localization length

$$\xi^{-1} = \ln(d_2) - \ln(d_1) \tag{23}$$

which was conjectured in [12] to describe the localization of the shock throughout the subphases $A_I$ and $B_I$. In fact, since the existence of a shock is a generic property of driven diffusive systems, our results support the picture developed in [14] where it is argued that a localization length of the form (23) is universal for driven diffusive systems in the subphases $A_I$ and $B_I$.

### *3.2. Branching–coalescing random walk (BCRW)*

In this case we have the following non-vanishing rates:

$$w_{34}, \quad w_{24}, \quad w_{42}, \quad w_{43}, \quad w_{32}, \quad w_{23}, \quad \alpha, \quad \gamma, \quad \beta. \tag{24}$$

In the periodic system there are two translation invariant stationary states in this model: Bernoulli measures with zero density and with a density $\rho^*$ respectively which depends only on the ratio

$$\frac{w_{24} + w_{34}}{w_{42} + w_{43}} = \frac{1-\rho^*}{\rho^*} \tag{25}$$

between the branching and coalescence rates. For the existence of diffusive shock measures in the open system one of the densities $\rho_i$ has to be zero, the other has to be $\rho^*$. Without loss of generality we set $\rho_2 = 0$. The non-vanishing rates then have to satisfy the conditions

$$w_{23} = \frac{1-\rho^*}{\rho^*} w_{43} \tag{26}$$

$$\gamma = \frac{1-\rho^*}{\rho^*}\alpha + (1-\rho^*)w_{32} - \frac{1-\rho^*}{\rho^*}w_{43} + \rho^* w_{34}. \tag{27}$$

This leaves seven free parameters.

Instead of the branching–coalescing random walk (BCRW) we could have chosen a birth–death-diffusion model with rates obtained from (25) and (26) by interchanging particles and vacancies. The densities behave under this transformation according to $\rho_i \to 1-\rho_i$ for $i = 1, 2$. As a microscopic shock position it is convenient to choose the position of the rightmost particle.

From (16) we obtain the shock hopping rates

$$d_1 = D_1 + w_{34}\rho^*/(1-\rho^*) \tag{28}$$

$$d_2 = w_{43}/\rho^*. \tag{29}$$

Hence the velocity of the shock

$$v_s = d_2 - d_1 \tag{30}$$

changes sign at hopping rates satisfying

$$D_{\mathrm{r}} = D_{\mathrm{l}}(1 - \rho^*) + w_{34}\rho^*. \tag{31}$$

This condition marks a field-driven first-order phase transition between the active state with density $\rho^*$ and the inactive state with zero density.

For a special tuning of the coalescence rates (instantaneous on-site coalescence which is equivalent to $D_{\mathrm{r}} = w_{24}$, $D_{\mathrm{l}} = w_{34}$) this process can be solved exactly with the help of the so-called inter-particle distribution functions (IPDF) [28, 34, 35], or, equivalently, using free fermion techniques, reviewed in detail in [9]. By passing to the continuum limit (lattice constant $a \to 0$) ben-Avraham [23] has shown for the free-fermion choice of coalescence rates with infinitesimal branching rate (proportional to the lattice constant) that the model has shock-like solutions if the initial state has zero density on one side and stationary density on the other side of the origin. He has also derived properties of higher order correlations which suggest the existence of a diffusive shock measure at least for this special limiting case of rates. Thus one has a picture comparable to the situation in the ASEP with the difference, however, that in the asymmetric exclusion process the densities on both sides of the shock are arbitrary while in the coalescence–branching model these densities are fixed to be zero and $\rho^* = \rho_1$, respectively. Moreover, in the limit of ben-Avraham the stationary density $\rho^*$ in the active domain is non-zero, but infinitesimal. Straightforwardly extending our result to the infinite system proves the existence of such a diffusive shock measure and shows that such a shock solution persists also for finite densities in the active domain.

We remark that for the case of symmetric hopping $D_{\mathrm{r}} = D_{\mathrm{l}}$, interesting macroscopic dynamics arise from (8) if we consider infinitesimal rates of branching and coalescence of the order of $a^2$ and also rescale time by $a^2$ (diffusive scale). We set

$$w_{24} = a^2\hat{w}_{24}, \quad w_{34} = a^2\hat{w}_{34}, \quad w_{42} = a^2\hat{w}_{42}, \quad w_{43} = a^2\hat{w}_{43} \tag{32}$$

and obtain within mean field theory

$$\frac{\partial\rho}{\partial t} = (D_{\mathrm{r}} + D_{\mathrm{l}})\frac{\partial^2\rho}{\partial x^2} + \hat{k}\rho(\rho^* - \rho) \tag{33}$$

with $\hat{k} = \hat{w}_{24} + \hat{w}_{34} + \hat{w}_{42} + \hat{w}_{43}$. This is the usual Fisher equation [3] which is also known to have travelling wave solutions similar to shocks.

Mean field theory for infinitesimal branching and coalescence rates, respectively, is justified since in this case the dynamics in any finite region are dominated by the pure exclusion process and hence is expected to be locally stationary and hence to have no correlations [17]. Neglecting correlations in the derivation of the hydrodynamic limit of (8) for the asymmetric process and keeping terms up to second order in the lattice constant one obtains

$$\frac{\partial\rho}{\partial t} = \nu\frac{\partial^2\rho}{\partial x^2} + \tilde{v}\frac{\partial\rho}{\partial x} - \tilde{\theta}\rho\frac{\partial\rho}{\partial x} + \tilde{k}\rho(\rho^* - \rho) \tag{34}$$

with infinitesimal viscosity $\nu = a(D_{\mathrm{r}} + D_{\mathrm{l}})$, single-particle velocity $\tilde{v} = D_{\mathrm{r}} - D_{\mathrm{l}} + a(\tilde{w}_{42} - \tilde{w}_{43})$, non-linearity $\tilde{\theta} = 2(D_{\mathrm{r}} - D_{\mathrm{l}}) + a(\tilde{w}_{42} + \tilde{w}_{24} - \tilde{w}_{43} - \tilde{w}_{34})$ and reaction constant $k = \tilde{w}_{42} + \tilde{w}_{24} + \tilde{w}_{43} + \tilde{w}_{34}$. This equation was studied by Murray [36] where it was shown that there are shock-like travelling wave solutions. For $a = 0$ the stationary equation reduces to an ordinary first order differential equation. With fixed boundary densities the solution can be obtained using the approach of [17].

### *3.3. Asymmetric Kawasaki–Glauber process (AKGP)*

In this case the non-zero rates are the death and branching rates as well as the one hopping rate where without loss of generality we consider non-vanishing hopping to the left

$$w_{12}, \quad w_{13}, \quad w_{42}, \quad w_{43}, \quad w_{32}, \quad \alpha, \quad \beta. \tag{35}$$

In the absence of diffusion ($w_{32} = 0$) this model is a variant of zero-temperature Glauber dynamics [26] with a non-vanishing magnetization current [37]. Including diffusion corresponds to a non-equilibrium coupling of the zero-temperature process to an infinite-temperature heat bath with asymmetric Kawasaki spin exchange dynamics. In a biological context branching corresponds to cell duplication by mitosis which can occur only if there is space available for a second cell. In this setting the death process describes the effect of certain types of drugs which kill both cells in the event of mitosis [38]. The two stationary densities are 0 and 1 respectively. The diffusive shock measures are of the same form as for the ASEP and BCRW respectively with $\rho_1 = 1$, $\rho_2 = 0$. Given an initial step function profile with a single domain wall ...1111100000... it is clear that the only events that can occur are the hopping of the domain wall to the right or left. Thus the domain wall performs a lattice random walk just as in the previous examples with hopping rates

$$d_1 = w_{13}, \qquad d_2 = w_{43} \tag{36}$$

to left ($d_1$) and right ($d_2$), respectively.

We remark that for a special choice of the branching rates $w_{43} = w_{12} - D_1$, $w_{42} = w_{13} + D_1$ the non-linear contribution to the equations of motion (8) vanishes identically [27]. Hence the *exact* evolution of the density profile is given by a lattice diffusion equation for all initial distributions. In this case the equations of motion for the density $\rho(x,t)$ do not give any indication of the existence of stable shocks. Hence the existence of a non-linearity in the dynamical equation for the density is not necessary for having shocks in the associated process.

## 4. ASEP with open boundaries

Here we wish to explore some of the ramifications of the results of the previous section on shock diffusion in the ASEP with open boundaries.

(1) As discussed above the stationary distribution of the shock position describes the steady state properties of the exclusion process with open boundaries along the manifold of boundary parameters defined by (19) and (20). The exact steady state properties of the exclusion process for all values of the boundary parameters may be calculated explicitly either by solving recursion relations [12] or by using the so-called matrix product approach [13] which involves the representation theory of a quadratic algebra equivalent to a $q$-deformed harmonic oscillator algebra [33]. The conditions (18)–(20) are equivalent to the conditions for the existence of a two-dimensional representation of the Fock-representation of the quadratic algebra used to calculate the stationary state properties of this model in [13, 39, 40]. This can be seen as follows; let us define the function $\kappa_+$ as:

$$\kappa_+(x, y) = \frac{-x + y + w_{23} - w_{32} + \sqrt{(-x + y + w_{23} - w_{32})^2 + 4xy}}{2x}. \tag{37}$$

Then the conditions (18)–(20) can be written in the form:

$$\rho_1 = \frac{1}{1+\kappa_+(\gamma,\alpha)} \tag{38}$$

$$\rho_2 = \frac{\kappa_+(\delta,\beta)}{1+\kappa_+(\delta,\beta)} \tag{39}$$

$$w_{23} = \kappa_+(\gamma,\alpha)\kappa_+(\delta,\beta)w_{32}. \tag{40}$$

We remind the reader that higher dimensional representations satisfy

$$(w_{23}/w_{32})^n = \kappa_+(\gamma,\alpha)\kappa_+(\delta,\beta), \tag{41}$$

for the derivation see [40].

(2) Diffusive shock measures have also been considered for the infinite system. This was done in [41] for discrete time evolution (parallel updating) and in [31] for continuous time evolution. The mathematical structure behind the one-particle nature of the bulk shock motion is the $U_q[SU(2)]$-symmetry of the generator of the ASEP with reflecting boundaries which relates one-particle states to shock states through the action of the ladder operator of $U_q[SU(2)]$. Surprisingly the open boundary conditions considered here break the symmetry, Yet the single-particle nature of the shock remains. This is reminiscent of partially broken symmetries observed in spin chains with diagonal boundary fields [42].

(3) In the infinite system consecutive multiple shocks which each satisfy (18) evolve according to $n$-particle dynamics, i.e. the $U_q[SU(2)]$-symmetry relates these $n$-shock measures to states with $n$ particles [31]. Using the ansatz discussed above it is easy to verify that by imposing the boundary conditions (41) required for the existence of $n$-dimensional representations of the stationary quadratic algebra, one also obtains closed equations of motion for shock measures in the open system. To see this one adopts a slightly different definition of the shock measure introduced in [31]: it is a product measure with density 1 at the shock positions $k_i$ and intermediate densities $\rho_i$ between sites $k_{i-1}, k_i$. The consecutive densities each satisfy (18), which by iteration leads to the condition (41) for the existence of $n$-dimensional representations of the stationary algebra. Hence the $n$-dimensional representations of the stationary algebra describe the stationary linear combination of shock measures with $n$ consecutive shocks. Notice that this modified definition of shock measures also allows for a representation of arbitrary shock measures (not satisfying any special relation between consecutive densities) in terms of linear combinations of the special shock measures.

(4) The definition of the shock position by the jump property of the shock measure (or the presence of a particle with probability 1 at the shock position in the alternative definition, respectively) is not a microscopic definition of the shock position for a single realization of the process. As the system evolves in time, one cannot trace the shock position to tell where exactly the shock is located. In a single realization the shock position would emerge only after spatial coarse graining. A convenient definition of the microscopic random position $X_t$ of the shock in a single realization of the process is the position of the *second-class particle* [43]–[45]. This particle behaves like an ordinary particle with respect to empty sites and like an empty site with respect to an ordinary particle. The second-class particle has a drift towards the shock [5] and its position may thus be defined as the position of the shock (cf [46] for this choice). Its diffusion coefficient has been obtained in [32]. The density

profile of the invariant shock measure as seen from the second-class particle was calculated in [47]. Its shape depends on the hopping ratio $q = \sqrt{D_r/D_l}$ and on the limiting densities. For limiting densities satisfying (18) the exact state is a pure Bernoulli shock measure with densities $\rho_1$ to left of the second-class particle and $\rho_2$ to its right. This observation suggests investigating the dynamics of shock measures with *second-class* particles at the shock positions.

We apply again the strategy of following the time evolution of shock measures by calculating the action of the Hamiltonian on the measure. In the infinite system one finds that indeed these measures form a closed sector analogous to $\mathcal{U}$ if the condition (18) is satisfied for consecutive shock densities. For the study of the open system we also need to define the properties of the second-class particle at the boundary sites. To this end we denote second-class particles by the symbol $B$ and explicitly consider reservoir sites $0$, $L+1$ which may either contain a $B$-particle with probability 1 or no $B$-particle, but an $A$-particle with probability $\rho_{1,2}$, respectively. We denote these two possible configurations of the boundary reservoir by $R_1$ and $B$ respectively and represent the left boundary processes as follows:

$$\begin{array}{ll}
R_1 0 \rightarrow R_1 A & \text{with rate } \delta_1 \rho_1 D_r \\
R_1 A \rightarrow R_1 0 & \text{with rate } \delta_1 (1-\rho_1) D_l \\
R_1 B \rightarrow BA & \text{with rate } \delta_1 \rho_1 D_r \\
R_1 B \rightarrow B0 & \text{with rate } \delta_1 (1-\rho_1) D_l \\
B0 \rightarrow R_1 B & \text{with rate } \delta_1 D_r \\
BA \rightarrow R_1 B & \text{with rate } \delta_1 D_l .
\end{array} \tag{42}$$

At the right boundary we define analogously two reservoir states $R_2$, $B$ respectively on site $L+1$ and allow for processes with rates

$$\begin{array}{ll}
0 R_2 \rightarrow A R_2 & \text{with rate } \delta_2 \rho_2 D_l \\
A R_2 \rightarrow 0 R_2 & \text{with rate } \delta_2 (1-\rho_2) D_r \\
B R_2 \rightarrow AB & \text{with rate } \delta_2 \rho_2 D_l \\
B R_2 \rightarrow 0B & \text{with rate } \delta_2 (1-\rho_2) D_r \\
0B \rightarrow B R_2 & \text{with rate } \delta_2 D_l \\
AB \rightarrow B R_2 & \text{with rate } \delta_2 D_r .
\end{array} \tag{43}$$

The number of $B$-particles is conserved in this dynamics. Physically this corresponds to the reflection of shocks at the boundaries in the open system. The first two transition rules for both boundaries which do not involve $B$-particles satisfy the injection/absorption rules (19), (20).

Considering the system with several $B$-particles one may study the time evolution of $n$ consecutive shocks with increasing densities at each point of discontinuity. For multiple shock measures with consecutive densities satisfying

$$\frac{D_r}{D_l} = \frac{\rho_{i+1}(1-\rho_i)}{(1-\rho_{i+1})\rho_i} \tag{44}$$

one finds $n$-particle dynamics. On the hydrodynamic scale $n$ consecutive shocks obey simple deterministic $n$-body dynamics: they move with constant speed until two shocks meet and then coalesce into a single shock. Thus after some time only one shock (the leftmost, which is the fastest) survives [48]. For the special family of boundary densities considered above this phenomenon can be studied on the lattice scale.

## 5. Conclusions

We have studied the dynamics of a class of reaction–diffusion processes with open boundaries on the *lattice scale* and established a complete list of models where exact travelling-shock solutions exist. For these systems we have detailed knowledge about the microscopic structure of the shock. We found that there are three families of such models: the ASEP, the BCRW, but on a more general manifold of parameters as considered previously, and a Kawasaki–Glauber spin-flip dynamics. In all three cases the time evolution of the shock measure is equivalent to that of a random walker on a lattice with $L + 1$ sites with homogeneous hopping rates in the bulk and special reflection rates at the boundary. The existence of such processes implies a rather remarkable property. Shocks behave like collective single-particle excitations already on the lattice scale—not only after coarse-graining where all the microscopic features of the shock are lost. The reduction of the exponentially large number of microscopic internal degrees of freedom $(2^L)$ to an only polynomial large number of macroscopically relevant degrees of freedom $(L+1)$ is not an uncontrolled and only phenomenologically motivated approximation, but an exact result on all scales of observation.

As is long known from zero-temperature Glauber dynamics, a hydrodynamic description of an interacting particle system in terms of a PDE for the particle density may fail to give any hint to the microscopic structure of the macroscopic solution even if the hydrodynamic equation is exact. Our results for the asymmetric Kawasaki–Glauber process (AKGP) indicate that this property is not a special feature only of Glauber dynamics. It remains as an open question under which general conditions and in which way the presence of a stable shock in a stochastic interacting particle system is reflected in the structure of the hydrodynamic limit. It also would be interesting to investigate travelling shocks in systems with defects, where, in the case of the ASEP, exact results are available for the steady state [49]–[52].

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