Nonequilibrium field-induced phase separation in single-file diffusion

Fatemeh Tabatabaei[1][†] and Gunter M. Schütz[2][†][‡]

†*Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany*

‡*Interdisziplinäres Zentrum für komplexe Systeme University of Bonn, Germany*

Using an analytically tractable lattice model for reaction-diffusion processes of hard-core particles we demonstrate that under nonequilibrium conditions phase coexistence may arise even if the system is effectively one-dimensional as e.g. in the channel system of some zeolites or in artificial optical lattices. In our model involving two species of particles a steady-state particle current is maintained by a density gradient between the channel boundaries and by the influence of an external driving force. This leads to the development of a fluctuating but always microscopically sharp interface between two domains of different densities which are fixed by the boundary chemical potentials. The internal structure of the interface becomes very simple for strong driving force. We calculate the drift velocity and diffusion coefficient of the interface in terms of the microscopic model parameters.

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[1]f.tabatabaei@fz-juelich.de

[2]g.schuetz@fz-juelich.de

1 Introduction

Diffusion of particles in long and narrow channels has a long history of the-
oretical investigation and has recently become a focus also of experimental
interest e.g. in the study of molecular diffusion in zeolites [1], diffusion of
colloidal particles in confined geometry [2] or optical lattices [3] and granular
diffusion [4]. In many such channel systems the particles cannot pass each
other. This mutual blocking phenomenon is known as single-file effect and
leads to subdiffusive behaviour [5, 6]. Among other things the single-file ef-
fect is responsible for low reaction effectivity in microporous catalysts [7] and
is thus of technical importance in chemical engineering. The single-file effect
occurs also in biological systems, examples being the motion of ribosomes
along the m-RNA during protein synthesis [8, 9] or transport by molecular
motors along microtubuli or actin filaments [10]. In single-file systems the
longitudinal motion is the most important dynamical mode and makes such
processes amenable to treatment by one-dimensional models [11, 12].

Low-dimensional diffusive particle systems are of great interest also from a
thermodynamic point of view. In open boundary systems, *kept far from equi-
librium* by maintaining a steady state particle current, various unexpected
kinds of critical phenomena have been discovered in recent years, includ-
ing boundary-induced phase transitions, phase separation and spontaneous
symmetry breaking, see [11, 12] and references therein for a review. These
finite-temperature critical phenomena have no counterpart in thermal equi-
librium since in one-dimensional systems with short range interactions there
is no mechanism that could prevent the creation and growth of an island of
the minority phase inside a domain of the majority phase. Therefore it is not

possible to have a phase-separated equilibrium state with a stable and microscopically sharp interface between two fluctuating domains characterized by different values of the order parameter.

Most of these nonequilibrium critical phenomena are not yet well-understood. Given the interesting diffusion properties as well as the potential for applications to catalytic reactions it would thus be interesting to explore critical phenomena in low-dimensional reaction-diffusion systems in more detail. Specifically, in this paper on one-dimensional reaction-diffusion systems we would like to investigate the existence and microscopic properties of interfaces between coexisting nonequilibrium domains which are macroscopically different.

In order to set the stage and sharpen the question we begin with some remarks of general nature and mention some results relevant to our approach. Systems of diffusing and reacting particles are usually described macroscopically by hydrodynamic equations for coarse-grained quantities like the particle density [13]. The density then represents the local order parameter specifying the spatial evolution of the macroscopic state of the system. Such equations are usually proposed on a phenomenological basis, paradigmatic examples being the Burgers equation for driven diffusive systems with particle conservation [14] or the Fisher equation for reactive systems without conservation law [15, 16]. 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. This means that in these systems phase separation may occur. The shock represents the interface between the two thermodynamically distinct

phases.

This hydrodynamic description of phase separation is, however, not fully satisfactory. It provides no insight into the microscopic origin of the phenomenon, and it gives no information about the internal structure of the shock. It could very well happen that in a particle system described on hydrodynamic (Eulerian) time scale by an equation which has shock solutions no corresponding microscopic discontinuity would be observable on less coarse-grained space or time scales which are experimentally relevant particularly for the quasi one-dimensional systems referred to above. In order to understand the structure of shocks and the emergence of such nonlinear behaviour from the microscopic laws that govern the stochastic motion and interaction of particles it is therefore necessary to *derive* the macroscopic equations from the microscopic dynamics rather than postulating them on phenomenological grounds.

Carrying out this programme starting from Newton's equation of motion constitutes a rather difficult problem. However, a substantial body of results of this nature has been obtained for specific one-dimensional stochastic lattice models [17, 18], the best-studied example being the asymmetric simple exclusion process (ASEP) [19, 20]. In this basic model for a driven diffusive system each site k on the infinite integer lattice $\mathbb{Z}$ 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_r and to the site $k - 1$ with rate D_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. For a single particle this is a biased random walk which on

large scales describes Brownian motion driven by a constant external force. The exclusion rule mimics a short-ranged hard-core interaction potential between particles. 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.

Moreover, there are a number of exact results about shocks in lattice gas models for driven diffusive systems [21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31], in reaction-diffusion systems [27, 31, 32, 33, 34, 35] (where shocks appear as Fisher waves on the macroscopic scale) and in spin-flip systems [27, 31, 35] where shocks correspond to domain walls [36]. It has emerged that in all these models the macroscopic shock discontinuity originates from a microscopically sharp increase of the local particle density, i.e., a decrease of the mean distance between particles that can be observed on the scale of a few lattice units (which typically represents the size of particles). The discontinuity itself performs a biased random motion with a constant mean speed and diffusive mean square displacement. The existence, structure, and dynamical properties of microscopically sharp shocks in lattice models for reaction-diffusion systems are the issues on which the present work focuses.

These results for the dynamical behaviour and microscopic properties of shocks have been obtained for infinite or periodic particle systems. In most 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 behavior of driven systems, even to the extent that boundary induced phase transitions between bulk states of different

densities occur [37, 38, 39]. 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 nonequilibrium phase diagram of driven diffusive systems with open boundaries, viz. phase transitions of first order, can be understood from the diffusive motion of shocks [40, 41], in analogy to the Zel'dovich theory of equilibrium kinetics of first-order transitions. In a series of recent papers [42, 43, 44, 45] these considerations, originally formulated for conservative dynamics, have been extended to non-conservative reaction-diffusion systems with open boundaries. As in equilibrium, the nonequilibrium theory of boundary-induced phase transitions requires the existence of shocks which are microscopically sharp. Therefore, the study of the microscopic structure of shocks in open systems is essential for understanding boundary-induced first order transitions and the phase separation phenomena associated with it.

After this survey we are finally in a position to precisely state the objective of this work. All the systems studied so far allow only for the presence of a single species of particles. No exact results have been reported so far for non-stationary travelling waves in open two-component systems, i.e. where two diffusive particles species A, B react with each other to form an inert reaction product or undergo a cracking or coagulation reaction ($B \rightleftharpoons 2A$). In order to address this question we adapt the strategy suggested in [27] to two-component systems: We take as initial distribution of particles a shock distribution with given microscopic properties and look for families of models

for which the shock distribution evolves into a linear combination of similar distributions with different shock positions. Thus the information of the microscopic structure of the shock that one has initially is preserved for all times. Remarkably it will transpire that such families of reaction-diffusion systems exist for strong external field that drives the particles and keeps them in a nonequilibrium state. We remark that in a similar treatment for a different family of two-component processes we have found such a phenomenon at some specific finite driving strength [46].

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 Sec. 3 we determine the families of models with travelling shock solutions on the finite lattice. In Sec. 4 we summarize our results and draw some conclusions. Some mathematical details of the calculations are given in the appendices.

2 Stochastic reaction-diffusion processes

2.1 Three-states lattice gas models

In order to keep the physics that lead to phase-separated nonequilibrium states as transparent as possible we study the simplest possible setting for a stochastic two-component reaction-diffusion process. We consider a lattice gas model defined on a lattice with L sites. The state of the system at any given time is described by a set of "occupation numbers" $\underline{n} = n_1, \ldots, n_L$ where $n_k = 0, 1, 2$ is the local occupation number at site k. These occupation numbers are abstract objects and serve as mathematical labels for three possible local states of each lattice site.

The bulk stochastic dynamics are defined by nearest neighbor transitions between the occupation variables which occur independently and randomly in continuous time after an exponentially distributed waiting time. The mean $\tau(n'_k, n'_{k+1}; n_k, n_{k+1})$ of this waiting time depends on the transition $(n_k, n_{k+1}) \rightarrow (n'_k, n'_{k+1})$. For later convenience we introduce an integer label

$$i = 3n_k + n_{k+1} + 1 \tag{1}$$

in the range $1 \leq i \leq 9$ for the occupation variables on two neighboring sites k and $k+1$. The inverse mean transition times are the transition rates w_{ij}. Here $i = 3n'_k + n'_{k+1} + 1$ labels the target configuration and j is the respective label of the initial configuration (n_k, n_{k+1}). We assume the bulk dynamics to be spatially homogeneous. The transition rates then do not explicitly depend on the site k.
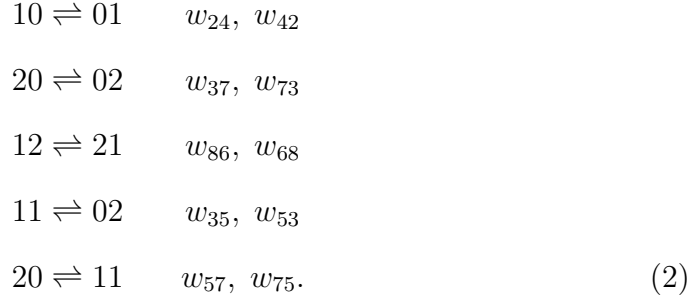
We require a single local conservation law where some linear function $C(n)$ of the local occupation numbers is conserved under the transitions [46]. It is straightforward to check that this allows for 10 nonvanishing rates w_{ij}. The physical interpretation of this conservation law as charge-, mass-, or particle conservation respectively depends on the physical interpretation of the occupation numbers n_k and will be given below. We present the following three families of models which are mathematically equivalent, but have rather different physical interpretations.

2.1.1 Diffusion without exclusion

In its most obvious interpretation the abstract occupation number n represents the number of particles on a given site. Requiring particle conservation

where $C(n) = n$ allows for 10 hopping processes with rates given as follows:

$$10 \rightleftharpoons 01 \qquad w_{24}, \; w_{42}$$

$$20 \rightleftharpoons 02 \qquad w_{37}, \; w_{73}$$

$$12 \rightleftharpoons 21 \qquad w_{86}, \; w_{68}$$

$$11 \rightleftharpoons 02 \qquad w_{35}, \; w_{53}$$

$$20 \rightleftharpoons 11 \qquad w_{57}, \; w_{75}. \tag{2}$$

Here there is no distinction between different particles, only the total number is recorded. Physically this process describes diffusion of a single species of particles in a pore system large enough to accommodate two particles in each pore. Thus the three states do not describe a two-component, single-file particle system, but a one-component system where particles can pass each other. This makes this process different from the previously studied two-state single-component systems which describe single-file diffusion [24, 26, 27]. For definiteness we shall focus in this paper on two-component reaction-diffusion systems and hence not make use of this one-component interpretation of the three local states.

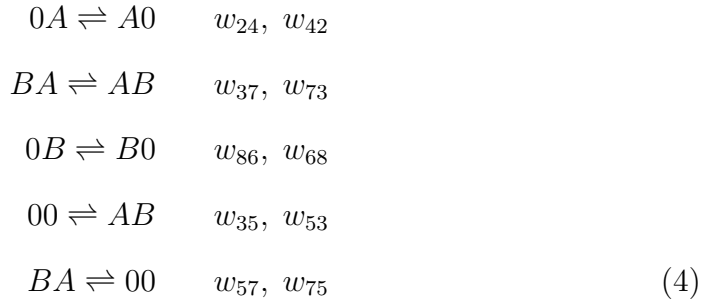### 2.1.2   Two-species annihilation $A + B \rightleftharpoons 0$

We define

$$C(n) = 1 - n \tag{3}$$

as charge associated with the state n of a lattice. The "occupation number" therefore denotes an internal degree of freedom in a single-file particle system. The value $n = 0$ corresponds to a positively charged particle (denoted as type A), $n = 1$ corresponds to a vacant site (denoted 0), and $n = 2$ corre-

sponds to occupation by a negatively charged particle (denoted as type B). As conservation law we require charge conservation, or, equivalently, conservation of the difference of particle numbers (of positively and negatively charged particles).

Since this process is mathematically equivalent to the particle conserving process (2) the dynamics of the process can be represented by the following ten transitions

$$0A \rightleftharpoons A0 \qquad w_{24}, \; w_{42}$$
$$BA \rightleftharpoons AB \qquad w_{37}, \; w_{73}$$
$$0B \rightleftharpoons B0 \qquad w_{86}, \; w_{68}$$
$$00 \rightleftharpoons AB \qquad w_{35}, \; w_{53}$$
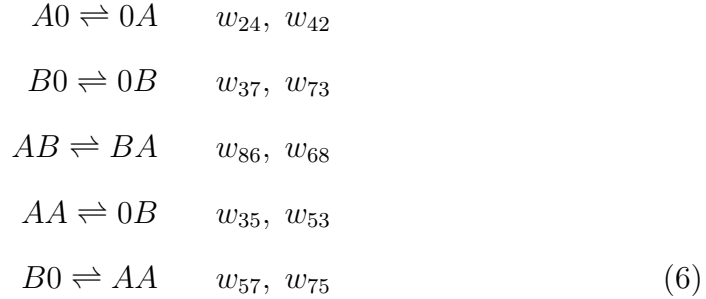$$BA \rightleftharpoons 00 \qquad w_{57}, \; w_{75} \tag{4}$$

This is the well-studied two-component creation/annihilation process, see [48] for a review of some important properties and experimental significance of the one-dimensional pure annihilation case. The main results of this paper are given in terms of this process.

2.1.3 Cracking $B \to 2A$

One may switch the role of A and 0. The "occupation number" $n = 0$ then corresponds to a vacant site 0, $n = 1$ corresponds to a particle of type A, and $n = 2$ corresponds to occupation by a particle of type B. We drop the assignment of charges to particles and instead introduce

$$C(n) = n =: M \tag{5}$$

as mass of the particles (in suitable units). A-particles thus have mass 1 and B-particles to have mass 2; the conservation law describes mass conservation. Under this mapping the process (4) read

$$
\begin{aligned}
A0 &\rightleftharpoons 0A & w_{24},\ w_{42} \\
B0 &\rightleftharpoons 0B & w_{37},\ w_{73} \\
AB &\rightleftharpoons BA & w_{86},\ w_{68} \\
AA &\rightleftharpoons 0B & w_{35},\ w_{53} \\
B0 &\rightleftharpoons AA & w_{57},\ w_{75}
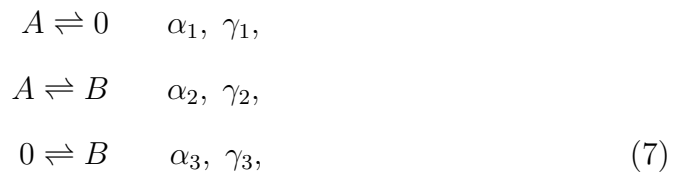\end{aligned}
\tag{6}
$$

The last two reactions corresponds to cracking of a molecule B with mass 2 into two identical parts A (mass 1 each), with coagulation as reversed process. The third process in this list is a recombination reaction between neighboring reactands.
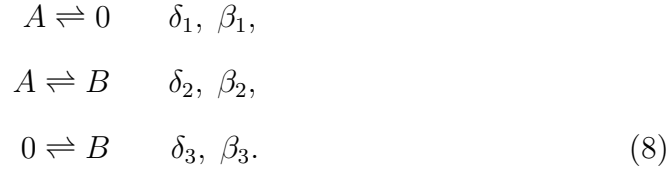
2.1.4 Boundary conditions and continuity equation

At the boundary sites $1, L$ we assume the system to be connected to some external reservoir with which the system can exchange particles. For definiteness we consider here and below charge conservation. The corresponding processes for mass conservation are obtained by changing $A \leftrightarrow 0$.

For injection and extraction of particles at the left boundary we introduce the rates :

$$
\begin{aligned}
A &\rightleftharpoons 0 & \alpha_1,\ \gamma_1, \\
A &\rightleftharpoons B & \alpha_2,\ \gamma_2, \\
0 &\rightleftharpoons B & \alpha_3,\ \gamma_3,
\end{aligned}
\tag{7}
$$

and for the right boundary

$$A \rightleftharpoons 0 \qquad \delta_1, \ \beta_1,$$

$$A \rightleftharpoons B \qquad \delta_2, \ \beta_2,$$

$$0 \rightleftharpoons B \qquad \delta_3, \ \beta_3. \tag{8}$$

Here and below the left rate refers to the process going from left to right, while the right rate is for the reversed process. The boundary rates are a further set of model parameters. Below we define them such that they are parametrized by 2 independent boundary chemical potentials which fix boundary densities for the conserved order parameter.

The presence of the bulk conservation law implies a lattice continuity equation

$$\frac{d}{dt}C_k = j_{k-1} - j_k \tag{9}$$

for the expectation $C_k = \langle\, C(n_k)\,\rangle$. This quantity plays the role of a conserved local order parameter. The quantity j_k is the current associated with the conservation law. It is given by the expectation of some combination of local occupation numbers, depending on the model under investigation, see below. Since we do not study here periodic systems we do not require the boundary sites where the system is connected to the reservoir to respect the conservation law. The quantities j_0, j_L entering the continuity equation for $k = 1$ and $k = L$ respectively are source terms resulting from the reservoirs. They are functions of the reservoir densities. The lattice continuity equation is the starting point for a coarse-grained hydrodynamic description of the time evolution of the local order parameter.

2.2 Master equation

The time evolution defined above can be written in terms of a continuous-time master equation for the probability vector

$$| P(t) \rangle = \sum_{\underline{n}} P(n_1, \cdots, n_L; t) | \underline{n} \rangle, \tag{10}$$

where $P(n_1, \cdots, n_L; t)$ is the distribution for the probability of finding particles at sites 1 to L and $| \underline{n} \rangle$ is the basis vector in the space of configurations [20]. The probability vector is normalized such that $\langle s|P \rangle = 1$ with the summation vector $\langle s | = \sum_{\underline{n}} \langle \underline{n} |$. The time evolution is generated by the stochastic Hamiltonian H whose offdiagonal matrix elements $H_{\underline{n}, \underline{n}'}$ are the negative transition rates between configurations. As required by conservation of probability, the diagonal elements are the negative sum of transition rates in the respective column.

Therefore the master equation is now described by the Schrödinger equation in imaginary time:

$$\frac{d}{dt} | P(t) \rangle = -H | P(t) \rangle. \tag{11}$$

with the formal solution

$$| P(t) \rangle = \mathrm{e}^{-Ht} | P(0) \rangle. \tag{12}$$

Since only nearest-neighbour interactions are included, the quantum Hamiltonian H defined above has the structure

$$H = b_1 + \sum_{k=1}^{L-1} h_{k,k+1} + b_L. \tag{13}$$

Here b_1 and b_L are the boundary matrices:

$$b_1 = - \begin{pmatrix} -(\alpha_1 + \alpha_2) & \gamma_1 & \gamma_2 \\ \alpha_1 & -(\gamma_1 + \alpha_3) & \gamma_3 \\ \alpha_2 & \alpha_3 & -(\gamma_2 + \gamma_3) \end{pmatrix}_1, \tag{14}$$

$$b_L = - \begin{pmatrix} -(\delta_1 + \delta_2) & \beta_1 & \beta_2 \\ \delta_1 & -(\beta_1 + \delta_3) & \beta_3 \\ \delta_2 & \beta_3 & -(\beta_2 + \beta_3) \end{pmatrix}_L. \tag{15}$$

The local bulk transition matrix $h_{k,k+1}$ with offdiagonal matrix elements $-w_{ij}$ acts non-trivially only on sites k and $k+1$. Below we give $h_{k,k+1}$ explicitly.

2.3 Nonequilibrium steady states

We stress that our family of models is defined in terms of transition rates, not in terms of an internal energy $E(\underline{n})$ that would determine the stationary distribution of the process as equilibrium distribution $P^*(\underline{n}) \propto \exp\left(-\beta E(\underline{n})\right)$. Instead, the stationary distribution is an *a priori* unknown and in general complicated function of the transition rates. It does not in general satisfy detailed balance and thus represents a nonequilibrium steady state. In order to be able to carry out explicit computations we restrict ourselves to systems such that the stationary distribution of the stochastic dynamics factorizes, i.e., one has a product measure without correlations between the occupation numbers at different sites.

Requiring the existence of a stationary product measure imposes constraints both on the boundary rates and on the bulk rates. Physically, the constraints on the boundary rates essentially means that the chemical potentials in the two reservoirs are equal, allowing the bulk to relax into a current-carrying stationary state with a chemical potential determined by the reservoirs. In this case the origin of the current is not a gradient in the external chemical potential of the reservoirs, but a constant bulk driving

force. The conditions on the bulk rates have a less transparent and model-dependent physical interpretation. Once these conditions are determined the model is fully defined and its stationary distribution is given for equal chemical potentials in the reservoir.

In the quantum Hamiltonian formalism introduced above a product measure is given by a tensor product

$$| P \rangle = |P_1) \otimes |P_2) \otimes ... \otimes |P_L).$$ (16)

Here the three-component single-site probability vectors $|P_k)$ has as its components the probabilities $P(n_k)$ of finding state n at site k. In the stationary distribution these probabilities are position-independent, $|P_k) \equiv |P)$, and the stationary probability vector thus has the form

$$| P^* \rangle = |P)^{\otimes L}.$$ (17)

By definition of stationarity the stationary probability vector satisfies the eigenvalue equation

$$H| P^* \rangle = 0.$$ (18)

We shall parametrize the one-site marginals $P(n_k)$ by a generalized fugacity z associated with the conserved quantity and an interaction parameter determined by the transition rates, see below. In formal analogy to equilibrium systems we shall refer to the logarithm of the fugacity as chemical potential.

2.4 Initial conditions

The objective of this paper is the analysis of the family of models which is defined by having a stationary product measure if the chemical potentials

in the reservoir are equal. However, as physical boundary conditions to be studied we envisage *different* chemical potentials in the reservoirs. The product measure is then no longer stationary and the questions arises what new properties the stationary distribution exhibits and how the system relaxes to its stationary distribution. Indeed, in order to avoid misunderstanding we stress that the product requirement on the stationary distribution with *equal* reservoir chemical potentials does not imply the absence of correlations during the time evolution of the more general open system with different reservoir chemical potentials.

Specifically, we prepare the system initially in a state described by a (nonstationary) shock measure of the form

$$| k \rangle = |P_1)^{\otimes k} \otimes |P_2)^{\otimes L-k}. \tag{19}$$

These shock measures have single-site probabilities given by $|P_1)$ in the left chain segment up to site k (chosen to match the chemical potential of the left reservoir) and single-site probabilities given by $|P_2)$ in the remaining chain segment from site $L-k$ up to site L (chosen to match the chemical potential at the right reservoir).

Such a shock measure defines fully the internal structure of the shock. Since there are no correlations in a shock measure one may regard the lattice unit as the intrinsic shock width. A typical configuration has a sharp decrease of the mean interparticle distance across the lattice point k. In the course of time the measure $| P(t) \rangle = \exp(-Ht)| k \rangle$ changes and it is interesting to investigate this time evolution. For the models studied below $| P(t) \rangle$ is computed explicitly and allows for a detailed explicit calculation of all correlations that develop with time.

3 Field-induced phase separation

3.1 Stationary distribution

Following the ideas outlined above we first search for stationary product solutions of the model with spatially constant single-site probabilities. By choosing the basis of three states as follows

$$|A) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |0) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |B) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \tag{20}$$

one can conveniently write the product measure for the periodic model in terms of a generalized fugacity z and arbitrary constant r

$$| P^* \rangle = \frac{1}{\nu^L} \begin{pmatrix} 1 \\ z \\ rz^2 \end{pmatrix}^{\otimes L} \tag{21}$$

Here

$$\nu = 1 + z + rz^2 \tag{22}$$

is the local "partition function". The quantity r parametrizes the density ratio of the two particle species, $\rho^B/\rho^A = rz^2$. The fugacity z is associated with the conservation law, i.e., in a periodic system where the charge is conserved $| P^* \rangle$ would be stationary for any value of z. This probability measure is grand-canonical. The charge $\sigma = \rho^A - \rho^B$ in this ensemble has mean

$$\sigma = 1 - z \frac{d}{dz} \ln \nu = \frac{1 - rz^2}{\nu}. \tag{23}$$

The corresponding canonical distributions with a definite value of the charge can be constructed in standard fashion, but we do not consider them here since we are dealing with an open system where the bulk fugacity is fixed

by the generalized chemical potentials of the reservoirs. The nonconserved particle density $\rho = \rho^A + \rho^B$ in this ensemble is given by

$$\rho = \frac{1 + rz^2}{\nu}. \tag{24}$$

The stationary distribution of the model is not known in full generality and we have to determine constraints on the bulk rates such that the product measure (21) is stationary. The transition matrix $h_{k,k+1}$ for the bulk stochastic dynamics is given by

$$-h_{k,k+1} =$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -w_{42} & 0 & w_{24} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -(w_{53} + w_{73}) & 0 & w_{35} & 0 & w_{37} & 0 & 0 \\ 0 & w_{42} & 0 & -w_{24} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & w_{53} & 0 & -(w_{35} + w_{75}) & 0 & w_{57} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -w_{86} & 0 & w_{68} & 0 \\ 0 & 0 & w_{73} & 0 & w_{75} & 0 & -(w_{37} + w_{57}) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & w_{86} & 0 & -w_{68} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}_{k,k+1}$$

$$\tag{25}$$

and stationarity of the product measure implies

$$h_{k,k+1} | P^* \rangle = [F(\hat{n}^A_{k+1} - \hat{n}^A_k) + F'(\hat{n}^B_{k+1} - \hat{n}^B_k)] | P^* \rangle. \tag{26}$$

Here F and F' are arbitrary constants and $\hat{n}^A_k$ and $\hat{n}^B_k$ are number operators which take value 1 if there is a particle of the respective species at site k and zero otherwise, i.e., $\rho^A = \langle n^A_k \rangle$ and $\rho^B = \langle n^B_k \rangle$ independently of k due to homogeneity of the measure.

In order to satisfy the relation (26) for systems with open boundaries we can write for b_1 and b_L, using another arbitrary constant g

$$b_1 | P^* \rangle = (F\hat{n}^A_1 + F'\hat{n}^B_1 + g) | P^* \rangle, \tag{27}$$

$$b_L | P^* \rangle = -(F \hat{n}_L^A + F' \hat{n}_L^B + g) | P^* \rangle. \tag{28}$$

As detailed in Appendix A one may solve the eigenvalue Eq. (18) and find F and F':

$$F = w_{24} - w_{42}, \tag{29}$$

$$F' = w_{86} - w_{68}. \tag{30}$$

Therefore the bulk rates and densities satisfy two relations due to the eigenvalue equation (18):

$$r = \frac{w_{35} + w_{75}}{w_{53} + w_{57}}, \tag{31}$$

$$w_{24} - w_{42} + w_{68} - w_{86} + w_{73} - w_{37} = \frac{w_{35}w_{57} - w_{53}w_{75}}{w_{35} + w_{75}}. \tag{32}$$

The first equation (31) expresses the constant r in terms of the reaction rates. The second equation (32) is a constraint on the transition rates which we impose on the model.

For the boundaries one needs to satisfy

$$g = \frac{1}{\nu}(F + F'rz^2). \tag{33}$$

This leaves two equations for the left boundary:

$$(w_{42} - w_{24})z(1+rz) - (w_{68} - w_{86})rz^2 + (\alpha_1 + \alpha_2)\nu - \gamma_1 z\nu - \gamma_2 rz^2\nu = 0, \tag{34}$$

$$(w_{68} - w_{86})rz^2(1+z) - (w_{42} - w_{24})rz^2 - \alpha_3 z\nu + (\gamma_3 + \gamma_2)rz^2\nu - \alpha_2\nu = 0, \tag{35}$$

and for the right boundary one has

$$(w_{42} - w_{24})z(1+rz) - (w_{68} - w_{86})rz^2 - (\delta_1 + \delta_2)\nu + \beta_1\nu + \beta_2\mu = 0, \tag{36}$$

$$(w_{68} - w_{86})rz^2(1+z) - (w_{42} - w_{24})rz^2 + \delta_3 z\nu - (\beta_3 + \beta_2)rz^2\nu + \delta_2\nu = 0. \tag{37}$$

These equations relate the boundary rates to the fugacity and moreover impose some constraints on the the boundary rates which are required for a proper interpretation as boundary reservoirs with fixed chemical potential.

We remark that the given choice of nonvanishing rates is only determined by the conservation law and requiring stationarity of the product measure. Many physical processes satisfy PT-invariance, i.e., the bulk dynamics should be symmetric under combined time reversal and space reflection. This physical input generalizes the equilibrium condition of detailed balance to allow for external driving forces. On the microscopic level of rates such driving forces lead to a bias in the hopping rates. Well-known examples for models of this kind are exclusion processes satisfying pairwise balance [47]. As in the more general case discussed so far, the system is forced into a nonequilibrium steady state with a stationary current flowing in the system. Following [46] we find that PT-invariance imposes the following further relations

$$w_{75} = rw_{53},$$
$$w_{35} = rw_{57}. \tag{38}$$

In the calculations of the next section we do not make use of these extra relations. We have merely listed them for possible applications of our general results to specific PT-symmetric systems.

3.2   Stationary Current and Hydrodynamics

As remarked above the conservation law implies a lattice continuity equation (9) for the charge current. To calculate the charge current we use the equation

of motion for the expected local charge density

$$\frac{d}{dt}\sigma_k(t) = \frac{d}{dt}[\langle n_k^A \rangle - \langle n_k^B \rangle] = j_{k-1} - j_k. \tag{39}$$

One finds for the expected local density of A-particles

$$
\begin{aligned}
\frac{d}{dt}\langle n_k^A \rangle = \quad & -w_{24}\langle n_{k-1}^0 n_k^A \rangle + w_{42}\langle n_{k-1}^A n_k^0 \rangle - w_{37}\langle n_{k-1}^B n_k^A \rangle + w_{73}\langle n_{k-1}^A n_k^B \rangle \\
& -w_{57}\langle n_{k-1}^B n_k^A \rangle + w_{75}\langle n_{k-1}^0 n_k^0 \rangle + w_{24}\langle n_k^0 n_{k+1}^A \rangle - w_{42}\langle n_k^A n_{k+1}^0 \rangle \\
& +w_{37}\langle n_k^B n_{k+1}^A \rangle - w_{73}\langle n_k^A n_{k+1}^B \rangle + w_{35}\langle n_k^0 n_{k+1}^0 \rangle - w_{53}\langle n_k^A n_{k+1}^B \rangle,
\end{aligned}
$$

$$\tag{40}$$

and for B-particles

$$
\begin{aligned}
\frac{d}{dt}\langle n_k^B \rangle = \quad & w_{37}\langle n_{k-1}^B n_k^A \rangle - w_{73}\langle n_{k-1}^A n_k^B \rangle - w_{86}\langle n_{k-1}^0 n_k^B \rangle + w_{68}\langle n_{k-1}^B n_k^0 \rangle \\
& +w_{35}\langle n_{k-1}^0 n_k^0 \rangle - w_{53}\langle n_{k-1}^A n_k^B \rangle - w_{37}\langle n_k^B n_{k+1}^A \rangle + w_{73}\langle n_k^A n_{k+1}^B \rangle \\
& +w_{86}\langle n_k^0 n_{k+1}^B \rangle - w_{68}\langle n_k^B n_{k+1}^0 \rangle - w_{57}\langle n_k^B n_{k+1}^A \rangle + w_{75}\langle n_k^0 n_{k+1}^0 \rangle
\end{aligned}
$$

$$\tag{41}$$

This gives the charge current

$$
\begin{aligned}
j_k = \quad & -w_{24}\langle n_k^0 n_{k+1}^A \rangle + w_{42}\langle n_k^A n_{k+1}^0 \rangle - 2w_{37}\langle n_k^B n_{k+1}^A \rangle + 2w_{73}\langle n_k^A n_{k+1}^B \rangle \\
& -w_{68}\langle n_k^B n_{k+1}^0 \rangle + w_{86}\langle n_k^0 n_{k+1}^B \rangle - w_{35}\langle n_k^0 n_{k+1}^0 \rangle + w_{53}\langle n_k^A n_{k+1}^B \rangle \\
& -w_{57}\langle n_k^B n_{k+1}^A \rangle + w_{75}\langle n_k^0 n_{k+1}^0 \rangle.
\end{aligned}
$$

$$\tag{42}$$

In the steady state we can compute the current using the stationary distribution. One finds

$$j^* = (-w_{24}+w_{42})\frac{z}{\nu^2} + [2(-w_{37}+w_{73})+w_{53}-w_{57}]\frac{rz^2}{\nu^2} + (w_{86}-w_{68})\frac{rz^3}{\nu^2} + (w_{75}-w_{35})\frac{z^2}{\nu^2}, \tag{43}$$

and by using (31) and the stationary condition (32)

$$j^* = \frac{1}{2}(w_{42} - w_{24})(\rho + \sigma)(1 - \sigma) + \frac{1}{2}(w_{86} - w_{68})(\rho - \sigma)(1 + \sigma), \qquad (44)$$

where σ and $\rho \equiv \langle n_k^A \rangle + \langle n_k^B \rangle$ are the stationary density of charges (23) and particles (24) respectively.

Since the individual particle densities are not conserved the equations of motion for the local densities take the form

$$\frac{d}{dt}\langle n_k^A \rangle = j_{k-1}^A - j_k^A + S_k, \qquad (45)$$

$$\frac{d}{dt}\langle n_k^B \rangle = j_{k-1}^B - j_k^B + S_k, \qquad (46)$$

with source term

$$
\begin{aligned}
S_k = \quad & -\tfrac{1}{2}w_{57}(\langle n_{k-1}^B n_k^A \rangle + \langle n_k^B n_{k+1}^A \rangle) + \tfrac{1}{2}w_{75}(\langle n_{k-1}^0 n_k^0 \rangle + \langle n_k^0 n_{k+1}^0 \rangle) \\
& + \tfrac{1}{2}w_{35}(\langle n_{k-1}^0 n_k^0 \rangle + \langle n_k^0 n_{k+1}^0 \rangle) - \tfrac{1}{2}w_{53}(\langle n_{k-1}^A n_k^B \rangle + \langle n_k^A n_{k+1}^B \rangle).
\end{aligned}
$$
$$(47)$$

The particle currents are given by

$$
\begin{aligned}
j_k^A = \quad & - w_{24}\langle n_k^0 n_{k+1}^A \rangle + w_{42}\langle n_k^A n_{k+1}^0 \rangle - w_{37}\langle n_k^B n_{k+1}^A \rangle + w_{73}\langle n_k^A n_{k+1}^B \rangle \\
& - \frac{1}{2}w_{35}\langle n_k^0 n_{k+1}^0 \rangle + \frac{1}{2}w_{53}\langle n_k^A n_{k+1}^B \rangle - \frac{1}{2}w_{57}\langle n_k^B n_{k+1}^A \rangle + \frac{1}{2}w_{75}\langle n_k^0 n_{k+1}^0 \rangle,
\end{aligned}
$$
$$(48)$$

$$
\begin{aligned}
j_k^B = \quad & w_{68}\langle n_k^B n_{k+1}^0 \rangle - w_{86}\langle n_k^0 n_{k+1}^B \rangle + w_{37}\langle n_k^B n_{k+1}^A \rangle - w_{73}\langle n_k^A n_{k+1}^B \rangle \\
& + \frac{1}{2}w_{35}\langle n_k^0 n_{k+1}^0 \rangle - \frac{1}{2}w_{53}\langle n_k^A n_{k+1}^B \rangle + \frac{1}{2}w_{57}\langle n_k^B n_{k+1}^A \rangle - \frac{1}{2}w_{57}\langle n_k^0 n_{k+1}^0 \rangle.
\end{aligned}
$$
$$(49)$$

The resulting charge current $j_k = j_k^A - j_k^B$ is studied above. One may introduce also a particle current $\tilde{j}_k = j_k^A + j_k^B$ and write

$$\frac{d}{dt}\rho_k(t) = \tilde{j}_{k-1} - \tilde{j}_k + 2S_k. \tag{50}$$

For a coarse-grained hydrodynamic description of the time-evolution of the system we follow standard arguments [17, 18]. We pass to a continuum description by making the lattice unit a (which until now had been taken to be $a = 1$) infinitesimal and we consider continuum space as $x = \frac{k}{L}$. The coarse-grained local observables $\sigma(x,t), \rho(x,t)$ in continuous space are averaged over a large but finite lattice interval around the lattice point x and therefore given by the expected local densities $\sigma_x(t), \rho_x(t)$. We consider Eulerian scaling $t' = ta$ with rescaled macroscopic time t'. In the continuum limit the two equations for σ and ρ then take the form (to leading order in the lattice constant a)

$$\partial_{t'}\sigma(x,t') = -\partial_x j(\sigma,\rho), \tag{51}$$

$$\partial_{t'}\rho(x,t') = -\partial_x \tilde{j}(\sigma,\rho) + R(\sigma,\rho)/a + \tilde{R}(\sigma,\rho), \tag{52}$$

where because of local stationarity

$$R(\sigma,\rho) = -\frac{1}{2}(w_{57} + w_{53})(\rho+\sigma)(\rho-\sigma) + 2(w_{75} + w_{35})(1-\rho)^2, \tag{53}$$

$$\tilde{R}(\sigma,\rho) = (w_{57} - w_{53})\frac{1}{4}[(\rho+\sigma)\partial_x(\rho-\sigma) - (\rho-\sigma)\partial_x(\rho+\sigma)]. \tag{54}$$

The space-time dependence of R and $\tilde{R}$ is implicit in arguments $\sigma(x,t'), \rho(x,t')$.

In this limit, when time and space are large, the term contained $R(\sigma,\rho)$ in the equation for ρ becomes large enough to make the two other terms negligible. Therefore $\rho(x,t)$ reaches its stationary state very fast, in agreement

with the notion that non-conserved local degrees of freedom have attained their stationary values under hydrodynamic scaling. This implies that in the stationary state $R(\sigma, \rho) = 0$, from which we obtain the stationary particle density

$$(\rho^{*2} - \sigma^2) = 4r(1 - \rho^*)^2. \tag{55}$$

for a given value of charge σ. Therefore ρ takes at any instant of (macroscopic) time a special value ρ^* which is a function of σ. The remaining slow dynamical mode is the charge, the evolution of which is thus governed by the hydrodynamic equation

$$\partial_{t'}\sigma(x, t') = -\partial_x j_x(\rho^*, \sigma) = -\partial_\sigma j(\rho^*, \sigma)\partial_x \sigma(x, t'). \tag{56}$$

In the second equation $j(\rho^*, \sigma)$ is the stationary current (44). This evolution equation is a nonlinear partial differential equation which can be solved by the method of characteristics. Because of the nonlinearity the solution may develop shocks in the charge distribution and we now turn to the investigation of these shocks on microscopic scale.

3.3 Shock measures

We assume that the initial distribution of charges exhibits a shock which on microscopic scale is represented by a shock measure (see Figure 1). We represent a shock measure with a shock in the fugacities between sites k and $k + 1$ as

$$| \, k \, \rangle = \frac{1}{\nu_1^k \nu_2^{L-k}} \begin{pmatrix} 1 \\ z_1 \\ rz_1^2 \end{pmatrix}^{\otimes k} \otimes \begin{pmatrix} 1 \\ z_2 \\ rz_2^2 \end{pmatrix}^{\otimes L-k}. \tag{57}$$

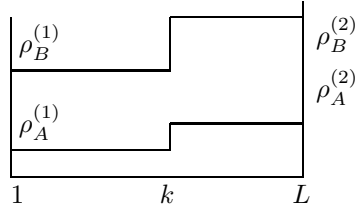In this model with open boundary condition, the first (second) fugacity matches the fugacity in left(right) boundary.

Figure 1: Coarse grained density profiles of a shock measure with shock between sites $k, k+1$.

Now we investigate the possibility that in analogy to the processes considered in [27, 35, 28] the family of shock measures $|k\rangle$ is closed under the time evolution t. This means that the initial measure evolves into a linear combination of shock measures after time t. This condition requires H which generates the time evolution to satisfy the following equation after an infinitesimal step

$$\frac{d}{dt}|k\rangle = d_1|k-1\rangle + d_2|k+1\rangle - (d_1 + d_2)|k\rangle. \tag{58}$$

We remark that this equation for the full particle distribution is mathematically equivalent to the evolution equation of a single-particle random walk with hopping rate d_1 to the left and d_2 to the right. Thus, if (58) can be satisfied, the shock in the initial distribution remains microscopically preserved at all times, but its position performs a random walk with shock hopping rates d_1 to the left and d_2 to the right respectively.

For further analysis we define

$$\tilde{h}_{i,i+1} \equiv h_{i,i+1} + F(n_i^A - n_{i+1}^A) + F'(n_i^B - n_{i+1}^B), \tag{59}$$

$$\tilde{b}_1 \equiv b_1 - Fn_1^A - F'n_1^B, \tag{60}$$

$$\tilde{b}_L \equiv b_L + Fn_L^A + F'n_L^B. \tag{61}$$

Using

$$\tilde{h}_{i,i+1}|\,k\,\rangle = 0 \quad for \ \ i \neq k, \tag{62}$$

$$\tilde{b}_1|\,k\,\rangle = g_1|\,k\,\rangle, \quad \tilde{b}_L|\,k\,\rangle = -g_2|\,k\,\rangle. \tag{63}$$

with

$$g_1 = -F\frac{1}{\nu_1} - F'\frac{rz_1^2}{\nu_1}, \tag{64}$$

$$g_2 = -F\frac{1}{\nu_2} - F'\frac{rz_2^2}{\nu_2}, \tag{65}$$

yields

$$-H|\,k\,\rangle = -(\sum_i \tilde{h}_{i,i+1} + \tilde{b}_1 + \tilde{b}_L)|\,k\,\rangle = (-\tilde{h}_{k,k+1} - g_1 + g_2)|\,k\,\rangle. \tag{66}$$

Together with (58) we thus find

$$(-\tilde{h}_{k,k+1} + d_1 + d_2 - g_1 + g_2)|\,k\,\rangle - d_1|\,k-1\,\rangle - d_2|\,k+1\,\rangle = 0. \tag{67}$$

The quantities $g_{1,2}$ are obtained from the boundary conditions (Appendix B).

This is a set 9 equations for the bulk rates. We have found a solution (see Appendix B) with $w_{24} = 0$. Putting this into the 9 equations (B-1)-(B-9) one finds after some straightforward algebra

$$d_2 = z_2 = 0, \tag{68}$$

$$d_1 = \frac{S}{\nu_1} = \frac{w_{42}}{\nu_1}, \tag{69}$$

$$w_{57} = w_{37} = 0, \tag{70}$$

$$w_{86} = w_{68}. \tag{71}$$

In this model there is a strong driving force for the positive particles that leads them to move only to the right as in the totally asymmetric simple

exclusion process. $z_2 = 0$ means that in the right branch of the shock the lattice is completely filled with positive particles (see Fig. 2). Hence incoming A-particles which react with B particles in the left branch of the shock hit the pure A-domain where they stop because of the single-file (exclusion) condition. The shock that separates the two domain moves only to the left with rate d_1. Hence its mean velocity v_s and diffusion coefficient D_s are determined by the density and hopping rate only of the A-particles in the left domain

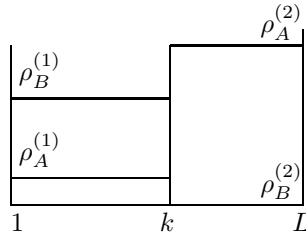$$v_s = 2D_s = w_{42}\rho_1^A. \tag{72}$$

Figure 2: Density profile of a shock measure in the case $z_2 = 0$

The interpretation of this result for the cracking process is readily available by interchanging the role of positive particles and vacancies. The right branch of the shock is the empty lattice where no reactions are going on. The left branch is active. All particles are driven to the left so that the inactive region grows diffusively with drift and fluctuations determined by (72) and ρ_1^A replaced by the vacancy density in the active domain.

We note that PT-invariance of the special model with $w_{24} = 0$ leads to

$$w_{35} = 0, \tag{73}$$

and to the stationary state condition

$$w_{42} = w_{73} + w_{53}. \tag{74}$$

The properties of the shock are not effected by PT-invariance.

4 Conclusions

We have studied the dynamics of a family of one-dimensional driven two-component reaction-diffusion processes with open boundaries on microscopic *lattice scale* and derived a hydrodynamic description on coarse grained Eulerian scale. This is the first main result, see Eqs. (44), (55), (56). The hydrodynamic equation is nonlinear and therefore admits shock solutions, corresponding to phase-separated states of the system. This generalizes one-dimensional field-induced phase separation that has been studied in some detail for lattice fluids in thermal equilibrium [49].

As the second main result we have obtained for a subset of models with very strong driving force detailed knowledge about the microscopic structure of the shock. The transition between the two phases is maximally sharp on lattice scale and the shock position performs a biased random walk with drift velocity and diffusion coefficient (72). Therefore, as observed in other models, 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. To our knowledge together with [46] these are the first results of this nature obtained for two-component reaction-diffusion processes. The mapping to different models, in particular to the partial exclusion process, suggests that this feature is not specific to single-file diffusion. The driving

force that is required to produce a maximally sharp interface depends on the model under consideration [46].

For a more general choice of rates the microscopic time evolution of the shock structure is more complicated. By analogy with general considerations of microscopic shock stability [20] and exact results for the asymmetric simple exclusion process [22] it is natural to expect a microscopically sharp interface, but with some extended structure that depends on the strength of the driving force. It would be very interesting to investigate experimentally in effectively one-dimensional driven reaction-diffusion systems with a conservation law the existence of field-induced phase separation and force-dependence of the internal width of the domain boundary.

Acknowledgments

Appendix A: Stationarity condition

Assuming product measure as stationary solution, we have

$$| P^* \rangle = \frac{1}{\nu^L} \begin{pmatrix} 1 \\ z \\ rz^2 \end{pmatrix}^{\otimes L}. \tag{A-1}$$

With (59)-(61), where n_i^A and n_i^B are number operators

$$n_i^A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_i, \qquad n_i^B = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}_i, \tag{A-2}$$

and eigenvalue equation

$$H| P^* \rangle = 0, \tag{A-3}$$

we write

$$\tilde{h}_{i,i+1}| P^* \rangle = (\tilde{b}_1 + \tilde{b}_L)| P^* \rangle = 0. \tag{A-4}$$

$\tilde{h}_{i,i+1}$ in terms of arbitrary constants F and F' is given by

$$\tilde{h}_{i,i+1} =$$

$$-\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -F-w_{42} & 0 & w_{24} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\Theta_1 & 0 & w_{35} & 0 & w_{37} & 0 & 0 \\
0 & w_{42} & 0 & F-w_{24} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & w_{53} & 0 & -(w_{35}+w_{75}) & 0 & w_{57} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & F'-w_{86} & 0 & w_{68} & 0 \\
0 & 0 & w_{73} & 0 & w_{75} & 0 & -\Theta_2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & w_{86} & 0 & -F'-w_{68} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}_{i,i+1},$$

$$\tag{A-5}$$

where

$$\Theta_1 = F - F' + w_{53} + w_{73}, \tag{A-6}$$

$$\Theta_2 = -F + F' + w_{37} + w_{57}. \tag{A-7}$$

Substituting $\tilde{h}_{i,i+1}$ in the Eq. (A-7) yields 5 independent equations. One gets F and F' by solving following equations

$$(F + w_{42} - w_{24})z = 0, \tag{A-8}$$

$$(-F' + w_{86} - w_{68})rz^2 = 0. \tag{A-9}$$

Hence F and F' are

$$F = w_{24} - w_{42}, \tag{A-10}$$

$$F' = w_{86} - w_{68}. \tag{A-11}$$

Three remained equations which have to be satisfied are

$$(w_{37} - \Theta_1)rz^2 + w_{35}z^2 = 0, \qquad (A\text{-}12)$$

$$(w_{73} - \Theta_2)rz^2 + w_{75}z^2 = 0, \qquad (A\text{-}13)$$

$$(w_{53} + w_{57})rz^2 - (w_{35} + w_{75})z^2 = 0. \qquad (A\text{-}14)$$

From Eq. (A-17) we obtain

$$r = \frac{w_{35} + w_{75}}{w_{53} + w_{57}}. \qquad (A\text{-}15)$$

Subtracting Eq. (A-15) from Eq. (A-16) yields second stationary state condition

$$w_{24} - w_{42} + w_{68} - w_{86} + w_{73} - w_{37} = \frac{w_{35}w_{57} - w_{53}w_{75}}{w_{35} + w_{75}}, \qquad (A\text{-}16)$$

where the sum of (A-15) and (A-16) is already satisfied.

This model is assumed to have open boundaries, therefore b_1 and b_L in terms of injection and extraction rates are given by Eq. (14) and Eq. (15). For satisfying Eq. (A-6) for the model with open boundaries one writes

$$b_1 | P^* \rangle = (F\hat{n}_1^A + F'\hat{n}_1^B + g)| P^* \rangle, \qquad (A\text{-}17)$$

$$b_L | P^* \rangle = -(F\hat{n}_L^A + F'\hat{n}_L^B + g)| P^* \rangle. \qquad (A\text{-}18)$$

where g is an arbitrary constant. Eq. (A-22) for the left boundary leads to three equations

$$(\alpha_1 + \alpha_2) - \gamma_1 z - \gamma_2 rz^2 = F + g, \qquad (A\text{-}19)$$

$$-\alpha_1 + (\gamma_1 + \alpha_3)z - \gamma_3 rz^2 = gz, \qquad (A\text{-}20)$$

$$-\alpha_2 - \alpha_3 z + (\gamma_2 + \gamma_3)rz^2 = (F' + g)rz^2. \qquad (A\text{-}21)$$

We then obtain g

$$
\begin{aligned}
g &= -\frac{F + F'rz^2}{\nu} \\
&= \gamma_1 + \alpha_3 - \frac{\alpha_1}{z} - rz\gamma_3.
\end{aligned}
$$

(A-22)

One also can obtain two conditions for boundary rates, which for the left one

$$(w_{42}-w_{24})z(1+rz)-(w_{68}-w_{86})rz^2+(\alpha_1+\alpha_2)\nu-\gamma_1 z\nu-\gamma_2 rz^2\nu = 0, \quad \text{(A-23)}$$

$$(w_{68}-w_{86})rz^2(1+z)-(w_{42}-w_{24})rz^2-\alpha_3 z\nu+(\gamma_3+\gamma_2)rz^2\nu-\alpha_2\nu = 0, \quad \text{(A-24)}$$

and for the right boundary

$$(w_{42} - w_{24})z(1 + rz) - (w_{68} - w_{86})rz^2 - (\delta_1 + \delta_2)\nu + \beta_1\nu + \beta_2\mu = 0, \quad \text{(A-25)}$$

$$(w_{68} - w_{86})\mu(1 - \mu) - (w_{42} - w_{24})\nu\mu - (\beta_3 + \beta_2)\mu + \gamma_3\lambda + \delta_2\nu = 0. \quad \text{(A-26)}$$

Appendix B: Random walk conditions for the shock

Explicitly the equations (67) that solve the random-walk condition for the shock are given by

$$
S - d_1\frac{\nu_1}{\nu_2} - d_2\frac{\nu_2}{\nu_1} = 0,
\tag{B-1}
$$

$$
(S - w_{35} - w_{75})z_1 z_2 + w_{53}rz_2^2 + w_{57}rz_1^2 - d_1\frac{\nu_1}{\nu_2}z_2^2 - d_2\frac{\nu_2}{\nu_1}z_1^2 = 0,
\tag{B-2}
$$

$$
S - d_1\frac{z_2^2}{z_1^2}\frac{\nu_1}{\nu_2} - d_2\frac{z_1^2}{z_2^2}\frac{\nu_2}{\nu_1} = 0,
\tag{B-3}
$$

$$
(S - w_{24})z_2 + w_{24}z_1 - d_1 z_2\frac{\nu_1}{\nu_2} - d_2 z_1\frac{\nu_2}{\nu_1} = 0,
\tag{B-4}
$$

$$
(S - w_{42})z_1 + w_{42}z_2 - d_1 z_2\frac{\nu_1}{\nu_2} - d_2 z_1\frac{\nu_2}{\nu_1} = 0,
\tag{B-5}
$$

$$(S - w_{68})z_2 + w_{68}z_1 - d_1\frac{z_2^2}{z_1}\frac{\nu_1}{\nu_2} - d_2\frac{z_1^2}{z_2}\frac{\nu_1}{\nu_2} = 0, \tag{B-6}$$

$$(S - w_{86})z_1 + w_{86}z_2 - d_1\frac{z_2^2}{z_1}\frac{\nu_1}{\nu_2} - d_2\frac{z_1^2}{z_2}\frac{\nu_1}{\nu_2} = 0, \tag{B-7}$$

$$(S - w_{37} - w_{53} - \Delta)rz_2^2 + w_{35}z_1z_2 + w_{37}rz_1^2 - d_1rz_2^2\frac{\nu_1}{\nu_2} - d_2rz_1^2\frac{\nu_2}{\nu_1} = 0, \tag{B-8}$$

$$(S - w_{73} - w_{57} + \Delta)rz_1^2 + w_{75}z_1z_2 + w_{73}rz_2^2 - d_1rz_2^2\frac{\nu_1}{\nu_2} - d_2rz_1^2\frac{\nu_2}{\nu_1} = 0, \tag{B-9}$$

where for compact notation we have introduced

$$S = d_1 + d_2 - g_1 + g_2; \quad \Delta = w_{24} - w_{42} + w_{68} - w_{86} + w_{73} - w_{37}. \tag{B-10}$$

These relations can be rewritten as 4 independent relations between the hopping rates and the fugacities

$$w_{24} = w_{68} \equiv p, \tag{B-11}$$

$$w_{42} = w_{86} \equiv q, \tag{B-12}$$

$$\frac{p}{q} = \frac{z_2^2}{z_1^2} \equiv X^2, \tag{B-13}$$

$$S = p + q. \tag{B-14}$$

and two equations for the shock hopping rates

$$d_1 = q\frac{\nu_2}{\nu_1}, \tag{B-15}$$

$$d_2 = p\frac{\nu_1}{\nu_2}. \tag{B-16}$$

To be more specific, solving Eq. (B-1) and (B-4)-(B-5) yields Eq. (B-15) and Eq. (B-16) for d_1 and d_2, from these two and Eq. (B-3) and (B-6)-(B-7), we obtain (B-13), a relation between rates and densities, then using Eq. (B-1) with above results yields Eq. (B-11), (B-12) and (B-14).

Using these 6 relations (B-11)-(B-16), equations (B-8), (B-9) and Eq. (B-2) respectively lead to the following relations for the so far undetermined rates

$$(p - q)(1 - \frac{w_{37}}{p})r + w_{35}(\sqrt{\frac{q}{p}} - 1) = 0, \tag{B-17}$$

$$(q - p)(1 - \frac{w_{73}}{q})r + w_{75}(\sqrt{\frac{p}{q}} - 1) = 0, \tag{B-18}$$

$$(p + q)r^{-1} + w_{53}(\sqrt{\frac{p}{q}} - 1) + w_{57}(\sqrt{\frac{q}{p}} - 1) = 0. \tag{B-19}$$

Simplifying Eq. (B-14) by using Eqs. (64)-(65) for g_1 and g_2 yields following more explicit relation between r and X

$$r = \frac{X}{(1 + X)^2}. \tag{B-20}$$

This relation on r together with Eqs. (B-17)-(B-19) and the stationary state equation (32), implies that $X = 0$. This solved by $p = z_2 = 0$.

The boundary equations (64)-(65) lead to

$$
\begin{aligned}
g_1 &= \frac{p - q}{\nu_1}(rz_1^2 - 1) \\
&= -\alpha_1 \frac{1}{z_1} - \gamma_3 r z_1 + (\gamma_1 + \alpha_3), \tag{B-21}
\end{aligned}
$$

$$
\begin{aligned}
g_2 &= \frac{p - q}{\nu_2}(rz_2^2 - 1) \\
&= \delta_1 \frac{1}{z_2} + \beta_3 r z_2 - (\beta_1 + \delta_2), \tag{B-22}
\end{aligned}
$$

for g_1 and g_2 respectively.

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