Multi-species reaction–diffusion models admitting shock solutions

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Abstract. A method for classifying n-species reaction–diffusion models admitting shock solutions is presented. The most general one-dimensional two-species reaction–diffusion model with nearest-neighbor interactions admitting uniform product measures as the stationary states is studied. Satisfying more constraints, these models may experience single-shock solutions. These models are generalized to multi-species models. The two-species models are studied in detail. Dynamical phase transitions of such models are also investigated.

Keywords: driven diffusive systems (theory), exact results, diffusion
1. Introduction

The stochastic modeling of systems is a useful method for studying the problems in non-equilibrium statistical physics. Reaction–diffusion systems are stochastic models which can be used to study the evolution of interacting particle systems. Extensive research has been done on one-dimensional reaction–diffusion systems, some of which belong to the emergence and evolution of shocks whose positions perform random walks, i.e. density discontinuities which are randomly on the move. The simplicity of the asymmetric simple exclusion process, including just diffusive processes, has provided researchers with a suitable baseline to take the first steps in exploring the dynamics of shocks [1]–[5]. In analogy to the asymmetric simple exclusion process (ASEP) some interesting models have been introduced, for example a driven diffusive two-channel system [6] or bricklayer’s model, which is a model without exclusion but yet uncorrelated [7,8]. To take into account systems including interacting processes, for instance, shock formation in driven diffusive systems containing homogeneous creation and annihilation of particles has been investigated [9,10] and more complicated systems have recently been described [12]–[16].

It is known that the ordinary Glauber model of a one-dimensional lattice with boundaries at any temperature shows a dynamical phase transition [18]. The dynamical phase transition is controlled by the rate of spin flip at the boundaries, and is a discontinuous change of the derivative of the relaxation time towards the stationary
configuration. In [19], using a transfer matrix method, it is shown that a one-dimensional kinetic Ising model with nonuniform coupling constants may exhibit a dynamical phase transition. Other phase transitions induced by boundary conditions have also been studied ([20]–[22] for example).

Our aim here is to introduce new solvable models. In [11] a single-species model with nearest-neighbor interactions on a one-dimensional lattice with open boundaries was considered. It was shown that there are three families of models with traveling wave solutions; the ASEP, the branching–coalescing random walk (BCRW) and the asymmetric Kawasaki–Glauber process (AKGP). A classification of single-species models with three-site interactions and special choice of symmetries has been studied in [12]. Recently some efforts have been made to obtain the models on a lattice with two types of particles and nearest-neighbor interactions. In [13] a model with diffusion and exchange processes was studied. In [14] a model with a degenerate conservation law and PT invariance (invariant under the application of time reversal and space reflection) was discussed. Another class of two-species models with a non-degenerate conservation law was presented in [15]. Besides the straightforward calculation of the master equation there is an alternative approach for dealing with reaction–diffusion problems—the so-called matrix product formalism. This is an algebraic method that takes advantage of non-commutative operators instead of probabilities. In [16] it is assumed that the density of A particles in a given site is proportional to the density of B particles at the same site. Using matrix product formalism, three three-state models were found which are basically two-state systems. One of these models is the generalization of [14].

In this paper there is an attempt to present a method for classifying $n$-species particle systems admitting single-shock solutions. In section 2, after a brief review of the formalism, a two-species reaction–diffusion model on a one-dimensional lattice with boundaries is introduced. In section 3, the most general two-species models with nearest-neighbor interactions, admitting uniform product measures as the stationary states, are studied. For such models reaction rates should satisfy some constraints. These conditions are obtained. In section 4, a single-shock measure is introduced and a classification method is presented. Then, it is generalized to multi-species models. In section 5, dynamical phase transitions of some two-species models are investigated. Finally, a discussion on the results of this paper and those of previous ones is presented.

2. Formulation

Two-species reaction–diffusion models with nearest-neighbor interactions on a one-dimensional lattice with $L$ sites are studied. There are two types of particles denoted by A and B. The processes are exclusive, which means that each site is either empty (this will be shown by $\emptyset$) or occupied by at most one particle, A or B. The empty state is denoted by $|\emptyset\rangle$, and the state occupied by particle A (B) is represented by $|A\rangle$ ($|B\rangle$). The three-dimensional vector space for each site is spanned by

\[
|\emptyset\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |A\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |B\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.
\] (1)
The $3^L$-dimensional vector space of the lattice is given by the tensor product of the single-site vector spaces $V^3$

$$V = V^3 \otimes \cdots \otimes V^3.$$ (2)

The state vector of the system is

$$|P\rangle_t = \sum_{\eta=1}^{3^L} P(\eta, t) |\eta\rangle,$$ (3)

where $|\eta\rangle$ is the basis vector of the lattice and $P(\eta, t)$ is the probability of finding the system in state $\eta$ in time $t$. Continuous-time Markovian evolution is the master equation

$$\frac{d|P\rangle_t}{dt} = H|P\rangle_t.$$ (4)

The non-diagonal elements of the generator $H$ are the transition rates $\omega_{ji}$, the transition rate from state $i$ to $j$, and its diagonal elements are the negative sum of the non-diagonal elements of their own columns. So the sum of each column is zero, and consequently

$$\langle S | H = 0,$$ (5)

where $\langle S \rangle$ is a row vector, all of whose elements are equal to 1. Let us denote $\omega_{i+1} := \sum_{j \neq i} \omega_{ji}$.

For a two-species model the local Hamiltonian $h_{k,k+1}$ is a $9 \times 9$ matrix, which acts on sites $k$ and $k + 1$, and contains 72 two-site transition rates. If the single-site states are respectively assumed empty ($\emptyset$), occupied by A and B the two-site states respectively become:

(1) $\emptyset \emptyset$ (4) $A \emptyset$ (7) $B \emptyset$
(2) $\emptyset A$ (5) $AA$ (8) $BA$
(3) $\emptyset B$ (6) $AB$ (9) $BB$. (6)

Let us assume open boundary conditions, where the particles can enter and leave the lattice from the first and last sites with the following rates

$$\alpha_{12} : A \rightarrow \emptyset, \quad \alpha_{21} : \emptyset \rightarrow A$$
$$\alpha_{13} : B \rightarrow \emptyset, \quad \alpha_{31} : \emptyset \rightarrow B$$ (7)

and change to each other with the rates

$$\alpha_{23} : B \rightarrow A, \quad \alpha_{32} : A \rightarrow B.$$ (8)

The Hamiltonians $B_1$ and $B_L$ are for the left and right boundaries and are in the form

$$B_{1/L} = \begin{pmatrix}
- (\alpha_{21}^{\ell/r} + \alpha_{31}^{\ell/r}) & \alpha_{12}^{\ell/r} & \alpha_{13}^{\ell/r} \\
\alpha_{21}^{\ell/r} & - (\alpha_{12}^{\ell/r} + \alpha_{32}^{\ell/r}) & \alpha_{13}^{\ell/r} \\
\alpha_{31}^{\ell/r} & \alpha_{23}^{\ell/r} & - (\alpha_{13}^{\ell/r} + \alpha_{23}^{\ell/r})
\end{pmatrix},$$ (9)

where the indices $\ell$ and $r$ stand for left and right. So the Hamiltonian for a one-dimensional $L$-site lattice with nearest-neighbor interactions and single-site interactions
at the boundaries is in the following form:

\[ H = B_1 \otimes \mathbb{I}^{(L-1)} + \sum_{k=1}^{L-1} \mathbb{I}^{(k-1)} \otimes h_{k,k+1} \otimes \mathbb{I}^{(L-k-1)} + \mathbb{I}^{(L-1)} \otimes B_L. \]  

(10)

\( \mathbb{I} \) denotes a \( 3 \times 3 \) unit matrix. We assume the interactions to be homogeneous, so \( h_{k,k+1} \) is the same for all sites. We also assume the interactions to be time independent.

3. Uniform product measures as stationary states

Let us consider the state vector of the system to be uncorrelated. Then the state of the system is the tensor product of the single-site state vectors

\[ |P\rangle = |P_1\rangle \otimes |P_2\rangle \otimes \cdots \otimes |P_L\rangle \]  

(11)

where \( |P_k\rangle \) is the state vector of site \( k \). If the occupation probability of particle A in site \( k \) is \( a_k \) and the occupation probability of particle B in site \( k \) is \( b_k \), the probability of being empty becomes \( 1 - (a_k + b_k) \). Consequently

\[ |P_k\rangle = \begin{pmatrix} 1 - (a_k + b_k) \\ a_k \\ b_k \end{pmatrix} \]  

(12)

where not only \( 0 \leq a_k, b_k \leq 1 \) but also \( 0 \leq a_k + b_k \leq 1 \). We also assume that the densities are uniform, and the state vector of each site is shown by \( |u\rangle \). Then the state vector of the lattice becomes

\[ |P\rangle = |u\rangle \otimes |U_L\rangle, \]  

(13)

which is a uniform product measure. The state vector \( |P\rangle \) is the stationary state of the system if

\[ H|P\rangle = 0, \]  

(14)

which gives

\[ H|u\rangle \otimes |U_L\rangle = 0. \]  

(15)

One can expand \( h|u\rangle \otimes |u\rangle \) in the following form

\[ h|u\rangle \otimes |u\rangle = A|u\rangle \otimes |u\rangle + \sum_{\mu, \nu=1}^{2} B_{\mu \nu}|x_\mu\rangle \otimes |x_\nu\rangle + \sum_{\mu=1}^{2} \{ C_\mu|u\rangle \otimes |x_\mu\rangle + D_\mu|x_\mu\rangle \otimes |u\rangle \}, \]  

(16)

where \( A, B_{\mu \nu}, C_\mu, \) and \( D_\mu \) are constant, and the two vectors \( |x_1\rangle \) and \( |x_2\rangle \) together with \( |u\rangle \) form a linearly independent set. Hence, substituting the above expansion into equation (15) leads to a combination of linearly independent terms. Thus, one deduces

\[ A = B_{\mu \nu} = 0, \quad C_\mu + D_\mu = 0. \]  

(17)

Therefore, for an infinite lattice or a periodic one, where there is no boundary term, equation (16) recasts to

\[ h|u\rangle \otimes |u\rangle = |u\rangle \otimes |x\rangle - |x\rangle \otimes |u\rangle, \]  

(18)
where the vector $|x\rangle$ is a linear combination of $|x_1\rangle$ and $|x_2\rangle$. This gives some constraints on the reaction rates. For a lattice with boundaries, $|u\rangle\otimes|L\rangle$ is a stationary uniform product measure provided that

$$h|u\rangle \otimes |u\rangle = |u\rangle \otimes |x\rangle - |x\rangle \otimes |u\rangle, \quad B_1|u\rangle = |x\rangle + |u\rangle, \quad B_L|u\rangle = -|x\rangle - |u\rangle,$$

where $\alpha$ is a constant, which depends on the reaction rates. Defining the vector $|\mathcal{R}\rangle$ by

$$|\mathcal{R}\rangle := h|u\rangle \otimes |u\rangle,$$

one obtains

$$R_1 = R_5 = R_9 = 0, \quad R_2 + R_4 = 0, \quad R_3 + R_7 = 0, \quad R_6 + R_8 = 0,$$

and

$$\frac{R_2}{u_1u_2} + \frac{R_6}{u_2u_3} = \frac{R_3}{u_1u_3}$$

(22)

where $R_i$ is the $i$th element of the vector $|\mathcal{R}\rangle$. Defining $\rho$ by

$$\rho := a + b.$$

Equation (21) may be written as

$$-\omega_1(1-\rho)^2 + (\omega_{12} + \omega_{14})(1-\rho)a + (\omega_{13} + \omega_{17})(1-\rho)b$$

$$+ (\omega_{16} + \omega_{18})ab + \omega_{15}a^2 + \omega_{19}b^2 = 0$$

(19)

$$\omega_{51}(1-\rho)^2 + (\omega_{52} + \omega_{54})(1-\rho)a + (\omega_{53} + \omega_{57})(1-\rho)b$$

$$+ (\omega_{56} + \omega_{58})ab - \omega_{55}a^2 + \omega_{59}b^2 = 0$$

$$\omega_{91}(1-\rho)^2 + (\omega_{92} + \omega_{94})(1-\rho)a + (\omega_{93} + \omega_{97})(1-\rho)b$$

$$+ (\omega_{96} + \omega_{98})ab + \omega_{95}a^2 - \omega_{9b}b^2 = 0$$

$$\omega_{21} + \omega_{41}(1-\rho)^2 + (-\omega_{12} + \omega_{14} + \omega_{32} - \omega_{42} - \omega_{44})(1-\rho)a$$

$$+ (\omega_{33} + \omega_{27} + \omega_{43} + \omega_{47})(1-\rho)b + (\omega_{25} + \omega_{45})a^2$$

$$+ (\omega_{26} + \omega_{28} + \omega_{46} + \omega_{48})ab + (\omega_{29} + \omega_{49})b^2 = 0$$

$$\omega_{31} + \omega_{71}(1-\rho)^2 + (\omega_{32} + \omega_{34} + \omega_{72} + \omega_{74})(1-\rho)a$$

$$+ (-\omega_{13} + \omega_{37} + \omega_{73} - \omega_{17})(1-\rho)b + (\omega_{35} + \omega_{75})a^2$$

$$+ (\omega_{36} + \omega_{38} + \omega_{76} + \omega_{78})ab + (\omega_{39} + \omega_{79})b^2 = 0$$

$$\omega_{61} + \omega_{81}(1-\rho)^2 + (\omega_{62} + \omega_{64} + \omega_{82} + \omega_{84})(1-\rho)a$$

$$+ (\omega_{63} + \omega_{67} + \omega_{83} + \omega_{87})(1-\rho)b + (\omega_{65} + \omega_{85})a^2$$

$$+ (-\omega_{66} + \omega_{68} + \omega_{86} - \omega_{68})ab + (\omega_{69} + \omega_{89})b^2 = 0.$$

(24)

These constraints guarantee the existence of a uniform product measure as a stationary state. Depending on the model, the stationary state may be unique. For such models, for any initial state, this product measure is the final state.

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4. Product shock measures

Let us assume that the occupation probability of particle A (B) in the first \( m \) sites is \( a_1 \) (\( b_1 \)) and in the latter \( (L - m) \) sites it is \( a_2 \) (\( b_2 \)). This is a single product shock measure, and the state vector is

\[
|e_m\rangle = |u\rangle \otimes |v\rangle \otimes (L-m)
\]

where

\[
|u\rangle = \left(\begin{array}{c} 1 - \rho_1 \\ a_1 \\ b_1 \end{array}\right), \quad |v\rangle = \left(\begin{array}{c} 1 - \rho_2 \\ a_2 \\ b_2 \end{array}\right).
\]

We briefly call it a shock measure. The shock state vectors \(|e_m\rangle, m = 0, 1, \ldots, L\) form \( L + 1 \) vectors and are a closed set under time evolution, if the evolution equations are in the form of

\[
H|e_m\rangle = d_1|e_{m-1}\rangle + d_2|e_{m+1}\rangle - (d_1 + d_2)|e_m\rangle, \quad 1 \leq m \leq L - 1,
\]

and

\[
H|e_0\rangle = D_1'|e_1\rangle - D_1'|e_0\rangle, \quad H|e_L\rangle = D_2'|e_{L-1}\rangle - D_2'|e_L\rangle.
\]

The shock position can perform one-site jumps with the rate \( d_1 \) (\( d_2 \)) to the left (right) and at the left (right) boundary with the rate \( D_1' \) (\( D_2' \)) to the right (left). As can be seen, the initial shock state can evolve into a linear combination of the shocks. It is said the shocks make an invariant sub-space. \( d_1, d_2, D_1', \) and \( D_2' \) are all non-negative and called the hopping rates of the shock position.

A shock is immobile when all the hopping rates \( d_1, d_2, D_1' \) and \( D_2' \) become zero. Then the shock does not move in the lattice, and the two stationary uniform product measures \(|e_0\rangle, |e_L\rangle\) are stationary.

4.1. Classification of shocks containing occupation probabilities different from 0 to 1

When there is a shock in the lattice, it is divided into two parts. The occupation probabilities for particles A and B in each part are \( a_k \) and \( b_k \), consequently \( 0 < a_k, b_k < 1 \). We also have \( 0 < \rho_k := a_k + b_k < 1 \). To have a shock, at least one of the particle densities in the first part of the lattice, \( a_1 \) or \( b_1 \), should be different from that in the other part. Here we have assumed that \( a_1 \neq a_2, b_1 \neq b_2 \), and \( \rho_1 \neq \rho_2 \). A shock measure is constructed of two stationary uniform product measures, so the reaction rates should satisfy two sets of the equations (21) and (22). To classify the shocks, we should first define equivalent models. One may obtain models which apparently seem to be different, but there exist transformations which relate them to each other. We take these models as equivalent models.

- Under the left and right exchange, some different models transform to each other so are equivalent.
The boundary rates together with the reaction rates satisfy these relations

\[ \rho = \frac{a_1}{a_2} \frac{b_1}{b_2} < \frac{1 - \rho_1}{1 - \rho_2} \]

\[ (K_1): \quad \frac{a_1}{a_2} = \frac{b_1}{b_2} < \frac{1 - \rho_1}{1 - \rho_2} \]

\[ (K_2): \quad \frac{a_1}{a_2} < \frac{b_1}{b_2} < \frac{1 - \rho_1}{1 - \rho_2} \]  (29)

So it is enough to study the cases \( K_1 \) and \( K_2 \).

4.1.1. \( K_1 \). Resulting from the condition \( a_1/a_2 = b_1/b_2 \), the non-zero reaction rates are

\[ \{ \omega_{23}, \omega_{24}, \omega_{27} \}, \quad \{ \omega_{56}, \omega_{58}, \omega_{59} \}, \]

\[ \{ \omega_{32}, \omega_{34}, \omega_{37} \}, \quad \{ \omega_{65}, \omega_{68}, \omega_{69} \}, \]

\[ \{ \omega_{42}, \omega_{43}, \omega_{47} \}, \quad \{ \omega_{85}, \omega_{86}, \omega_{89} \}, \]

\[ \{ \omega_{72}, \omega_{73}, \omega_{74} \}, \quad \{ \omega_{95}, \omega_{96}, \omega_{98} \}, \]  (30)

in which particles A and B can convert to each other, but no particle can annihilate to an empty state. Thus the total number of empty sites and consequently the total number of particles are conserved in the bulk. This model is symmetric under the transformation A \( \leftrightarrow \) B. As will be seen, the relations we obtain reflect this symmetry. We have

\[ (\omega_{56} + \omega_{58})a_1b_1 - \omega_{59}b_1^2 = 0, \]

\[ (\omega_{96} + \omega_{98})a_1b_1 + \omega_{95}a_1^2 - \omega_{99}b_1^2 = 0, \]

\[ \frac{\omega_{32} + \omega_{34} + \omega_{72} + \omega_{74}}{\omega_{23} + \omega_{43} + \omega_{27} + \omega_{47}} = \frac{b_1}{a_1} \]

\( d_1 \) is given by

\[ d_1 = \frac{a_1}{a_2} \left( \frac{\omega_{24} + \omega_{27}}{a_1} b_1 \right) = \frac{a_1}{a_2} \left( \omega_{37} + \omega_{34} a_1 \right) b_1 \]

\[ = \frac{1 - \rho_1}{1 - \rho_2} \left( \omega_{42} + \omega_{43} b_1 \right) a_1 \]

\[ = \frac{1 - \rho_1}{1 - \rho_2} \left( \omega_{73} + \omega_{72} a_1 \right) b_1. \]  (32)

\( d_1 \) and \( d_2 \) are related to each other through

\[ \frac{d_1}{(1 - \rho_1)a_1} = \frac{d_2}{(1 - \rho_2)a_2}. \]  (33)

The boundary rates together with the reaction rates satisfy these relations

\[ \rho_1((\omega_{32} + \omega_{72})a_1 - (\omega_{23} + \omega_{43})b_1) \]

\[ = (\omega_{56} + \omega_{58} + \omega_{65} + \omega_{86} + \omega_{69} + \omega_{89})a_1b_1 + \omega_{65}a_1^2 + \omega_{69}b_1^2 \]

\[ = (\alpha_1^\ell - \alpha_{13}^\ell)a_1b_1 - (\omega_{32}^\ell a_1 + \omega_{32}^\ell b_1) \rho_1, \]  (34)

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$d_1$ and $d_2$ can be described by boundary rates through

$$d_1 = \frac{-(\alpha_{21}^\ell + \alpha_{31}^\ell)(1 - \rho_1) + \alpha_{12}^\ell a_1 + \alpha_{13}^\ell b_1}{\rho_1 - \rho_2},$$

$$d_2 = \frac{(\alpha_{21}^r + \alpha_{31}^r)(1 - \rho_2) - \alpha_{12}^r a_2 - \alpha_{13}^r b_2}{\rho_1 - \rho_2},$$

(35)

and also

$$\alpha_{21}^\ell/r b_1 = \alpha_{31}^\ell/r a_1.\tag{36}$$

Defining $\alpha_{ij}^{\ell+r} := \alpha_{ij}^\ell + \alpha_{ij}^r$, one arrives at

$$(\alpha_{12}^{\ell+r} - \alpha_{13}^{\ell+r})a_2 = (-\alpha_{32}^{\ell+r} + \alpha_{23}^{\ell+r} b_2)\frac{\rho_2}{b_2}.$$  

(37)

And finally the rates $D_1', D_2'$ are

$$D_1' = d_2 - d_1 a_2 a_1 + \frac{\alpha_{21}^\ell}{a_1} = d_2 a_2 - a_1 + \frac{\alpha_{12}^\ell a_1 + \alpha_{13}^\ell b_1}{(1 - \rho_1)\rho_1},$$

$$D_2' = d_1 - d_2 a_1 a_2 + \frac{\alpha_{31}^\ell}{a_2} = d_1 a_1 - a_2 + \frac{\alpha_{13}^r b_2 + \alpha_{12}^r a_2}{(1 - \rho_2)\rho_2}.\tag{38}$$

Setting all the transition rates equal to zero except for the diffusion rates $\omega_{73}, \omega_{37}, \omega_{12}, \omega_{24}$ and the exchange rates $\omega_{86}, \omega_{68}$, the results of [13] can be obtained:

$$\omega_{68} = \omega_{86}, \quad \omega_{24} = \omega_{37} = d_1 a_2 a_1, \quad \omega_{42} = \omega_{73} = d_1 \frac{(1 - \rho_2)}{(1 - \rho_1)} \tag{39}$$

$$\frac{d_1}{(1 - \rho_1)\rho_1} = \frac{d_2}{(1 - \rho_2)a_2} \tag{40}$$

$$\alpha_{21}^{\ell/r} b_1 = \alpha_{31}^{\ell/r} a_1,$$

$$(\alpha_{12}^{\ell/r} - \alpha_{13}^{\ell/r}) a_1 b_1 = (-\alpha_{32}^{\ell/r} + \alpha_{23}^{\ell/r} b_1)\rho_1,$$

$$d_1 = \alpha_{31}^{\ell} (1 - \rho_1) - \alpha_{32}^{\ell} a_1 + (\alpha_{13}^{\ell} + \alpha_{23}^{\ell}) b_1 \tag{41}$$

$$d_2 = \frac{\alpha_{31}^{r} (1 - \rho_2) + \alpha_{32}^{r} a_2 - (\alpha_{13}^{r} + \alpha_{23}^{r}) b_2}{b_1 - b_2}$$

$$D_1' = (\omega_{42} - \omega_{24})\rho_2 + \frac{\alpha_{31}^{\ell}}{b_1} = (\omega_{24} - \omega_{42})(1 - \rho_2) + \frac{\alpha_{13}^{r} b_1 + \alpha_{12}^{r} a_1}{(1 - \rho_1)\rho_1},$$

$$D_2' = (\omega_{24} - \omega_{42})\rho_1 + \frac{\alpha_{31}^{r}}{b_2} = (\omega_{42} - \omega_{24})(1 - \rho_1) + \frac{\alpha_{13}^{r} b_2 + \alpha_{12}^{r} a_2}{(1 - \rho_2)\rho_2}.\tag{42}$$

It is seen that the rates of diffusion for both particles A and B are the same as obtained in [11] for a single-species model. So ASEP is a special example of the case $K_1$.

The shock will be immobile ($d_1 = d_2 = D_1' = D_2' = 0$) if

$$\omega_{24}, \omega_{12}, \omega_{37}, \omega_{72}, \omega_{34}, \omega_{43}, \omega_{37}, \omega_{73} = 0.$$  

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These reactions are

\[
\emptyset A \leftrightarrow A \emptyset \\
\emptyset A \leftrightarrow B \emptyset \\
\emptyset B \leftrightarrow B \emptyset \\
\emptyset B \leftrightarrow A \emptyset.
\]

(44)

The above transition rates are responsible for particle transportation from one site to another. Whenever these rates are non-zero, the shock position moves. Thus, to fix the shock position, these rates should be zero. We also have

\[
\alpha_{12}^b, \alpha_{15}^b, \alpha_{21}^b, \alpha_{31}^b = 0.
\]

(45)

These boundary rates should be zero to maintain the total number of particles in the bulk. So we have

\[
\frac{\omega_{32} + \omega_{74}}{\omega_{23} + \omega_{47}} = \frac{b_1}{a_1} \quad \omega_{32} a_1 - \omega_{23} b_1 = \alpha_{32}^b a_1 - \alpha_{23}^b b_1 \quad (\alpha_{32}^b + \alpha_{32}^r) a_2 = (\alpha_{23}^b + \alpha_{23}^r) b_2.
\]

(46)

The other relations remain unchanged.

4.1.2. \(K_2\). In this model the occupation probabilities should satisfy the following relation:

\[
\frac{(1 - \rho_1) a_1}{b_1^2} = \frac{(1 - \rho_2) a_2}{b_2^2}.
\]

(47)

Then the non-zero transition rates are

\[
\omega_{24}, \omega_{29}, \omega_{32}, \omega_{42}, \omega_{92}, \omega_{94}, \omega_{37}, \omega_{73}, \omega_{68}, \omega_{86}.
\]

(48)

Therefore, besides the diffusion (\(\omega_{24}, \omega_{42}, \omega_{37}, \omega_{73}\)) and exchange processes (\(\omega_{68}, \omega_{86}\)), provided that (47) is satisfied, the processes \(\emptyset A \leftrightarrow BB\) and \(A \emptyset \leftrightarrow BB\) are also allowed. The occupation probabilities should also satisfy the following relation:

\[
\frac{a_1(1 - \rho_2) - a_2(1 - \rho_1)}{b_1(1 - \rho_2) - b_2(1 - \rho_1)} = \frac{a_1 b_2 - a_2 b_1}{a_1(1 - \rho_2) - a_2(1 - \rho_1)}.
\]

(49)

This relation should be held in order to guarantee the possibility of the simultaneous existence of the two uniform parts in the bulk. Then we have

\[
\omega_{37} = \omega_{86}, \quad \omega_{73} = \omega_{68},
\]

(50)

\[(\omega_{92} + \omega_{94})(1 - \rho_1) a_1 - (\omega_{29} + \omega_{49}) b_1^2 = 0,
\]

d_1 and d_2 are connected through

\[
\frac{d_1}{(1 - \rho_1) a_1} = \frac{d_2}{(1 - \rho_2) a_2}
\]

(51)

d_1 is given by

\[
d_1 = \frac{a_1}{a_2} \omega_{37} = \frac{(1 - \rho_1)}{(1 - \rho_2)} \frac{a_1}{a_2} \left( \omega_{24} + \omega_{29} \frac{b_1 a_1 - a_2}{a_1 \rho_1 - \rho_2} \right) = \frac{(1 - \rho_1)}{(1 - \rho_2)} \left( \omega_{42} + \omega_{49} \frac{b_2 a_1 - a_2}{a_2 \rho_1 - \rho_2} \right) = \frac{(1 - \rho_1) a_1}{a_1 b_2 - a_2 b_1} \left( \omega_{92} \frac{a_2}{b_2} - \omega_{94} \frac{a_1}{b_1} \right).
\]

(52)
Defining $\alpha^t_{ij} + \alpha^r_{ij} =: \alpha^t_{ij}$, then $D'_1, D'_2$ will be
\begin{align}
D'_1 &= \frac{1}{b_2 - b_1} \left( -\alpha^t_{31}(1 - \rho_2) - \alpha^t_{32}a_2 + (\alpha^t_{13} + \alpha^t_{23})b_2 \right) \\
D'_2 &= \frac{1}{b_2 - b_1} \left( \alpha^t_{31}(1 - \rho_1) + \alpha^t_{32}a_1 - (\alpha^t_{13} + \alpha^t_{23})b_1 \right).
\end{align}

(53)

The boundary relations have been included in the appendix. A question which may arise is: is there any solution for these sets of conditions? These conditions are some constraints on the reaction rates, and occupation probabilities of the particles, $a_i$ and $b_i$, which should be checked. In addition to these equations, there are also some inequalities; reaction rates should be non-negative and $0 \leq a_i, b_i \leq 1$. It is difficult to check all these analytically. We have solved numerically these sets of equations and inequalities. It is seen that there are solutions for these sets of equations. So all the conditions on the parameters can be fulfilled simultaneously.

This case does not have a similar one-species model. To have a one-species analogue, the processes in which all the three single-site states are involved should vanish, i.e. the processes $\emptyset \leftrightarrow BB$ should not happen. This means that just the diffusion and exchange transition rates can be held, which leads to a contradiction to the inequality $a_1/a_2 < b_1/b_2 < (1 - \rho_1)/(1 - \rho_2)$.

4.1.3. Generalization to more than two species. Let us consider an $n$-species system. The local Hamiltonian $h$, acting on two adjacent sites, is an $(n+1) \times (n+1)$ matrix. We assume a single-shock measure consisting of the single-site state vectors $|u\rangle$ and $|v\rangle$. It can be seen from the equations (10) and (27) that if the equations governing the evolution of $h|u\rangle \otimes |u\rangle, h|u\rangle \otimes |v\rangle$ and $h|v\rangle \otimes |v\rangle$ are given, the dynamics of the shock in the bulk of the lattice is fully determined. To facilitate the calculation, we choose a new basis like $\zeta = \{|u\rangle, |v\rangle, |x_1\rangle, \ldots, |x_{n-1}\rangle\}$, where $|x_i\rangle$s are arbitrary vectors ineffective in the final results. Adopting the same strategy as section 3, from expanding the three vectors $h|u\rangle \otimes |u\rangle, h|u\rangle \otimes |v\rangle$ and $h|v\rangle \otimes |v\rangle$ in the new basis and then substituting these expansions into (27), one obtains the following equations for the uniform parts of the shock
\begin{align}
\langle h|u\rangle \otimes |u\rangle &= E_1(\langle u\rangle \otimes \langle v\rangle - \langle v\rangle \otimes \langle u\rangle) + \sum_{\mu=1}^{n-1} E_{\mu+1}(\langle u\rangle \otimes \langle x_\mu\rangle - \langle x_\mu\rangle \otimes \langle u\rangle), \\
\langle h|v\rangle \otimes |v\rangle &= -F_1(\langle v\rangle \otimes \langle u\rangle - \langle u\rangle \otimes \langle v\rangle) + \sum_{\mu=1}^{n-1} F_{\mu+1}(\langle v\rangle \otimes \langle x_\mu\rangle - \langle x_\mu\rangle \otimes \langle v\rangle),
\end{align}

(54)

and the following equation for the shock position
\begin{align}
\langle h|u\rangle \otimes |v\rangle &= (d_2 - F_1)(\langle u\rangle \otimes \langle u\rangle - \langle u\rangle \otimes \langle v\rangle) + (d_1 - E_1)(\langle v\rangle \otimes \langle v\rangle - \langle u\rangle \otimes \langle v\rangle) \\
&+ \sum_{\mu=1}^{n-1} F_{\mu+1}|u\rangle \otimes |x_\mu\rangle - \sum_{\mu=1}^{n-1} E_{\mu+1}|x_\mu\rangle \otimes |v\rangle.
\end{align}

(55)
$E$ s and $F$ s are some constants depending on the reaction rates and probabilities. When all the occupation probabilities are different from 0 and 1, the equations (54) seem to be sufficient to determine the non-zero rates. In this case, the equation (55) for the shock position either manages to link the two uniform parts or completely fails and rejects the validity of the whole model.

The equations (54) are both in the following form

$$h|w\rangle \otimes |w\rangle = |w\rangle \otimes |x\rangle - |x\rangle \otimes |w\rangle.$$  

We define $|\mathcal{R}\rangle := h|w\rangle \otimes |w\rangle$ whose elements are $R_k$s. We have obtained some relations for these elements by generalizing our previous knowledge of what these relations are for one- and two-species systems, (21). We have

$$R_{(\xi - 1)(n + 1) + \xi} = 0, \quad \xi = 1, \ldots, n + 1.$$  

(57)

These relations belong to the two-site states in which either both sites are empty or they are occupied by particles of the same type, for example $\emptyset\emptyset$ or AA. We also have

$$R_{(\psi - 1)(n + 1) + \phi} + R_{(\phi - 1)(n + 1) + \psi} = 0,$$

$$\begin{cases} \psi \neq \phi, \\ \psi = 1, \ldots, n \\ \phi = 2, \ldots, n + 1. \end{cases}$$  

(58)

Each relation of this kind is related to those two-site states which are the mirror of each other, for example $\emptyset A$ and $A\emptyset$.

It is known that in the case of single-species models there is only one model with $0 < \rho < 1$, admitting shock as a random walker [11]. This model is the ASEP. For the two-species case, we have found two models here. One of these models is a generalization of the ASEP, and the other one has no single-species analogue.

Let us consider a three-species model. The single-site states, respectively, are an empty site denoted by $\emptyset$ and sites occupied by A, B and C. Then the two-site states become:

$$\begin{align*}
(1) & \emptyset\emptyset & (5) & A\emptyset & (9) & B\emptyset & (13) & C\emptyset \\
(2) & \emptyset A & (6) & AA & (10) & BA & (14) & CA \\
(3) & \emptyset B & (7) & AB & (11) & BB & (15) & CB \\
(4) & \emptyset C & (8) & AC & (12) & BC & (16) & CC
\end{align*}$$  

(59)

and the equations (57) and (58) give

$$R_1 = R_6 = R_{11} = R_{16} = 0$$

$$R_2 + R_5 = 0, \quad R_3 + R_9 = 0, \quad R_4 + R_{13} = 0$$

$$R_7 + R_{10} = 0, \quad R_8 + R_{14} = 0, \quad R_{12} + R_{15} = 0.$$  

(60)

To make a classification, one should compare the following quantities with each other

$$\begin{align*}
\frac{(1 - \rho_1)^2}{(1 - \rho_2)^2} & \quad \frac{a_1^2}{a_2^2} & \quad \frac{b_1^2}{b_2^2} & \quad \frac{c_1^2}{c_2^2} & \quad \frac{(1 - \rho_1)a_1}{(1 - \rho_2)a_2} \\
\frac{(1 - \rho_1)b_1}{(1 - \rho_2)b_2'} & \quad \frac{(1 - \rho_1)c_1}{a_2b_2'} & \quad \frac{a_1c_1}{a_2c_2'} & \quad \frac{b_1c_1}{b_2c_2'}
\end{align*}$$  

(61)
where \(a, b\) and \(c\) are the occupation probabilities of particles and \(\rho\) is defined as \((\rho := a + b + c)\). These parameters are suitable criteria for the ratio of the number of the two-site states of the two uniform parts. As we know, the greater the number of a definite two-site state is, the more likely an associated process is to happen. Therefore, the reason why the parameters (61) are helpful for introducing tractable models is that they can be used to control the processes in the lattice. Since the parameters (61) are the square or product of the parameters \(\frac{a_1}{a_2}, \frac{b_1}{b_2}, \frac{c_1}{c_2}\) and \((1 - \rho_1)/(1 - \rho_2)\), it will be easier to first compare these parameters.

Three distinct models will be obtained for a three-species lattice:

- The cases with one inequality like
  \[
  \frac{a_1}{a_2} = \frac{b_1}{b_2} = \frac{c_1}{c_2} < \frac{(1 - \rho_1)}{(1 - \rho_2)}. \tag{62}
  \]
  For this case, the non-zero transition rates are
  \[
  \omega_{ij}, \quad i \neq j, \quad i, j = 6, 7, 8, 10, 11, 12, 14, 15, 16,
  \]
  \[
  \omega_{lk}, \quad l \neq k, \quad l, k = 2, 3, 4, 5, 9, 13 \tag{63}
  \]
  in which particles A, B and C can convert to each other, but the number of empty sites is conserved. Resulting from (62), this model is invariant under the transformations \(A \leftrightarrow B\), \(A \leftrightarrow C\) and \(C \leftrightarrow B\). It shows that, from the four single-site states of this case, the states A, B and C are similar to each other. Another model of this type is
  \[
  \frac{a_1}{a_2} = \frac{b_1}{b_2} < \frac{c_1}{c_2} = \frac{(1 - \rho_1)}{(1 - \rho_2)}. \tag{64}
  \]
  The non-zero transition rates are
  \[
  \omega_{ef}, \quad e \neq f, \quad e, f = 2, 3, 5, 8, 9, 12, 14, 15,
  \]
  \[
  \omega_{gh}, \quad g \neq h, \quad g, h = 6, 7, 10, 11,
  \]
  \[
  \omega_{op}, \quad o \neq p, \quad o, p = 1, 4, 13, 16. \tag{65}
  \]
  This model has the symmetries \(A \leftrightarrow B\) and \(C \leftrightarrow \emptyset\), so the states A with B and empty site with C are similar to each other. Therefore, for the cases with one inequality, one expects an analogous single-species model, resembling a reduction of two in the number of particles.

- The cases with two inequalities like
  \[
  \frac{a_1}{a_2} = \frac{b_1}{b_2} < \frac{c_1}{c_2} < \frac{(1 - \rho_1)}{(1 - \rho_2)}. \tag{66}
  \]
  This model has the symmetry \(A \leftrightarrow B\), thus it is expected to have a similar two-species model, resembling a reduction of one in the number of particles. The non-zero transition rates are
  \[
  \omega_{4,13}, \omega_{13,4}, \omega_{i',j'}, \quad i' \neq j', \quad i', j' = 6, 7, 10, 11,
  \]
  \[
  \omega_{l',k'}, \quad l' \neq k', \quad l', k' = 8, 12, 14, 15,
  \]
  \[
  \omega_{e',f'}, \quad e' \neq f', \quad e', f' = 2, 3, 5, 9, 16 \tag{67}
  \]
Multi-species reaction–diffusion models admitting shock solutions

in which, besides the diffusion and exchange processes, particles \( A \) and \( B \) can convert to each other and the processes \((\emptyset A, A \emptyset, B \emptyset, B \emptyset \leftrightarrow CC)\) are also possible provided that the following relation is satisfied

\[
\frac{(1 - \rho_1)a_1}{(1 - \rho_2)a_2} = \frac{c_2^2}{c_1^2}.
\]

(68)

There is another essential condition for the occupation probabilities, which is

\[
((a_1 + b_1)(1 - \rho_2) - (a_2 + b_2)(1 - \rho_1))^2
= (c_1(1 - \rho_2) - c_2(1 - \rho_1))(a_1 + b_1)c_2 - (a_2 + b_2)c_1).
\]

(69)

This relation comes from equation (55) for the shock position.

- The cases with three inequalities like

\[
\frac{a_1}{a_2} < \frac{b_1}{b_2} < \frac{c_1}{c_2} < (1 - \rho_1)
\]

(70)

are expected to be originally three-species models. The non-zero transition rates are

- \( \omega_{7,10}, \omega_{10,7}, \omega_{4,13}, \omega_{13,4}, \)
- \( \omega_{g'g'}, g' \neq h', g', h' = 2, 5, 12, 15, \)
- \( \omega_{o'o'}, o' \neq p', o', p' = 8, 11, 14, \)
- \( \omega_{q'q'}, q' \neq s', q', s' = 3, 9, 16 \)

(71)

with the conditions

\[
\frac{(1 - \rho_1)a_1}{(1 - \rho_2)a_2} = \frac{b_1c_1}{b_2c_2}, \quad \frac{(1 - \rho_1)b_1}{(1 - \rho_2)b_2} = \frac{c_2^2}{c_1^2}, \quad \frac{a_1c_1}{a_2c_2} = \frac{b_1^2}{b_2^2}.
\]

(72)

In this case, besides the diffusion and exchange processes, resulting from the above relations, the processes \((\emptyset A, A \emptyset \leftrightarrow BC, CB), (\emptyset B, B \emptyset \leftrightarrow CC)\) and \((AC, AC \leftrightarrow BB)\) are also allowed. The occupation probabilities should also satisfy another relation coming from equation (55).

Accordingly for \( n \)-species systems, it is expected to find \( n \) distinct models. One for which there is a similar single-species model, one with a two-species analogue, . . . , and finally there is an \( n \)-species model which has no \( k \)-species analogue with \( k < n \).

4.2. Shocks containing the occupation probabilities 0 and 1

Now, we study the shocks in which some parts of the lattice are empty (or equivalently completely occupied).

4.2.1. \( \rho_1 \neq 0, 1, \rho_2 = 0 \). Assume \( a_2 = b_2 = 0 \) and \( a_1, b_1 \neq 0, 1 \). In this case, \( \omega_{i1} = 0 \) to prevent particle production in the empty part of the shock, and subsequently \( \omega_{i1} = 0 \), otherwise all the two-site states can convert to \( \emptyset \emptyset \) but there is no way to leave this state. All the other remaining rates can be non-zero. Besides the relations (21) for \( \rho_1, b_1, a_1, \)

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the other relations are as follows. The parameters $d_1, d_2$ are given by

\[
d_1 = \frac{1}{a_1}[(\omega_{42} a_1 + \omega_{33} b_1)(1 - \rho_1) + (\omega_{46} + \omega_{48}) a_1 b_1 + \omega_{45} a_1^2 + \omega_{49} b_1^2] \\
= \frac{1}{b_1}[(\omega_{72} a_1 + \omega_{73} b_1)(1 - \rho_1) + (\omega_{76} + \omega_{78}) a_1 b_1 + \omega_{75} a_1^2 + \omega_{79} b_1^2],
\]

\[
d_2 = \frac{1}{(1 - \rho_1) a_1}(-\omega_{24} a_1 + \omega_{27} b_1) = \frac{1}{(1 - \rho_1) b_1}(\omega_{34} a_1 + \omega_{37} b_1) \\
= \frac{1}{a_1}[(\omega_{54} a_1 + \omega_{57} b_1) = \frac{1}{a_1 b_1}(\omega_{64} a_1 + \omega_{67} b_1) \\
= \frac{1}{b_1 a_1}(\omega_{84} a_1 + \omega_{87} b_1) = \frac{1}{b_1}(\omega_{94} a_1 + \omega_{97} b_1).
\]

The boundary rates together with the reaction rates satisfy these relations

\[
(\alpha_{12}^\ell - \alpha_{13}^\ell) a_1 b_1 + (\alpha_{32}^\ell a_1 - \alpha_{23}^\ell b_1) \rho_1 = (-\omega_{4+} a_1 + \omega_{47} b_1 + d_2 a_1) \rho_1 \\
= [(\omega_{62} + \omega_{64}) a_1 + (\omega_{63} + \omega_{67}) b_1](1 - \rho_1) + \omega_{65} a_1^2 + \omega_{69} b_1^2 \\
+ (-\omega_{6+} + \omega_{68}) a_1 b_1,
\]

and we have

\[
-d_2 \rho_1(1 - \rho_1) + d_1 \rho_1 = -(\alpha_{21}^\ell + \alpha_{31}^\ell)(1 - \rho_1) + \alpha_{12}^\ell a_1 + \alpha_{13}^\ell b_1.
\]

Particles should not enter the right boundary, so $\alpha_{31}^r = \alpha_{21}^r = 0$. The relations between the boundary rates are

\[
\alpha_{21}^r b_1 = \alpha_{31}^r a_1.
\]

Using the definition $\alpha_{ij}^{\ell+r} := \alpha_{ij}^{\ell} + \alpha_{ij}^r$, one arrives at

\[
(\alpha_{12}^{\ell+r} - \alpha_{13}^{\ell+r}) a_1 b_1 = (-\alpha_{32}^{\ell+r} a_1 + \alpha_{23}^{\ell+r} b_1) \rho_1.
\]

$D_1'$, $D_2'$ are

\[
D_1' = \frac{\alpha_{12}^{\ell}}{b_1}, \quad D_2' = d_1 - d_2(1 - \rho_1) + \frac{\alpha_{12}^r a_1 + \alpha_{13}^r b_1}{\rho_1}.
\]

The shock will be immobile if all the transition rates from the fourth and seventh rows and columns of $h$ except for $\omega_{47}, \omega_{74}$ become zero, i.e. the processes starting from (ending at) the states $A\emptyset, B\emptyset$ which make the shock position move to the right (left). Also the following rates at the boundaries should be zero:

\[
\alpha_{21}^\ell = \alpha_{31}^\ell = \alpha_{12}^\ell = \alpha_{13}^\ell = \alpha_{12}^r = \alpha_{13}^r = 0
\]

which means no particles enter or leave the boundaries. The other relations will remain unchanged.

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4.2.2. $\rho_1 = 1, \rho_2 = 0$. Consider $a_2 = b_2 = 0$ and $a_1 + b_1 = 1$. We assume $a_1, b_1 \neq 0, 1$ to have a two-species model. The non-zero transition rates are

\[
\begin{pmatrix}
\omega_{12} & \omega_{13} & \omega_{14} & \omega_{17} \\
\omega_{23} & \omega_{22} & \omega_{32} & \omega_{47} \\
\omega_{32} & \omega_{53} & \omega_{54} & \omega_{56} \\
\omega_{62} & \omega_{63} & \omega_{64} & \omega_{65} \\
\omega_{72} & \omega_{73} & \omega_{74} & \omega_{85} \\
\omega_{82} & \omega_{83} & \omega_{84} & \omega_{85} \\
\omega_{92} & \omega_{93} & \omega_{94} & \omega_{95} \\
\omega'_{14} & \omega'_{17} & \omega'_{23} & \omega'_{47} \\
\end{pmatrix}
\]

There are no constraints on $\omega_{i2}$ and $\omega_{i3}$. One should expect this, because the states ($\emptyset$A) and ($\emptyset$B) do not exist in the final state. We also have

\[
(\omega_{56} + \omega_{58})a_1 b_1 - \omega_{+5} a_1^2 + \omega_{59} b_1^2 = 0
\]

\[
(\omega_{96} + \omega_{98})a_1 b_1 + \omega_{95} a_1^2 - \omega_{-4} b_1^2 = 0.
\]

$d_1, d_2$ are given by

\[
d_1 = \omega_{14} a_1 + \omega_{17} b_1
\]

\[
d_2 = \frac{1}{a_1^2} (\omega_{54} a_1 + \omega_{57} b_1) = \frac{1}{a_1 b_1} (\omega_{64} a_1 + \omega_{67} b_1)
\]

\[
= \frac{1}{b_1 a_1} (\omega_{84} a_1 + \omega_{87} b_1) = \frac{1}{b_1^2} (\omega_{94} a_1 + \omega_{97} b_1).
\]

The following relations should also be satisfied by reaction rates

\[
\alpha_{22} a_1 - \alpha_{23} b_1 = (-\omega_{+6} + \omega_{68}) a_1 b_1 + \omega_{65} a_1^2 + \omega_{69} b_1^2
\]

\[
= (d_2 + d_1) a_1 - \omega_{+4} a_1 + \omega_{47} b_1.
\]

The left part of the shock should be fully occupied, so $\alpha'_{12} = \alpha'_{13} = 0$ and the right part of the shock should be empty, thus $\alpha'_{21} = \alpha'_{31} = 0$. The relations between the boundary rates are

\[
\alpha'_{23} b_1 = \alpha'_{31} a_1
\]

\[
(\alpha'_{12} - \alpha'_{13}) a_1 b_1 = -(\alpha'_{32} + \alpha'_{32}) a_1 + (\alpha'_{23} + \alpha'_{23}) b_1.
\]

$D'_1, D'_2$ are given by

\[
D'_1 = \frac{\alpha'_{31}}{b_1} \quad D'_2 = \alpha'_{12} a_1 + \alpha'_{13} b_1.
\]

The shock will be immobile if we eliminate the processes (A$\emptyset$, B$\emptyset$ $\rightarrow$ $\emptyset$0), i.e. $\omega_{14} = \omega_{17} = 0$, to prevent the shock position from moving to the left, and also the processes (A$\emptyset$, B$\emptyset$ $\rightarrow$ AB, BA, AA, BB) should vanish to prevent the shock position from moving to the right, i.e. the transition rates $\omega_{47}, \omega_{74}$ are the only non-zero rates of the fourth and seventh columns of $h$. The following boundary rates should be also zero:

\[
\alpha'_{21} = \alpha'_{31} = \alpha'_{12} = \alpha'_{13} = 0
\]

which means no particle can enter or leave the boundaries.
Some other shapes of the shocks for two-species systems can also be predicted:

\[
\begin{align*}
(a_1 = 0, a_2 \neq 0, 1, b_1 \neq 0, 1, b_2 = 0) \\
(a_1 = 0, a_2 \neq 0, 1, b_1 = 1, b_2 = 0) \\
(a_1 \neq 0, 1, a_2 \neq 0, 1, b_1 \neq 0, 1, b_2 = 0, a_1 + b_1 \neq 0, 1) \\
(a_1 \neq 0, 1, a_2 \neq 0, 1, b_1 \neq 0, 1, b_2 = 0, a_1 + b_1 = 1).
\end{align*}
\]

It can be shown that the models with \(a_1 = a_2, (a_1, a_2 \neq 0, 1), b_1 \neq b_2, (b_1, b_2 \neq 0, 1)\) and \(\rho_1, \rho_2 \neq 0, 1\) do not exist.

5. Dynamical phase transition for two-species models

In this section dynamical phase transition for the three cases \(K_1, (\rho_1 \neq 0, 1, \rho_2 = 0)\), and \((\rho_1 = 1, \rho_2 = 0)\) is studied. In [17], phase transition in single-species models possessing shock solutions is studied. It will be shown that there are three phases. For some region of the parameter space, the relaxation time is independent of the reaction rates at the boundaries. Changing continuously the reaction rates at the boundaries, there is a point where the relaxation time begins changing, so that at this point there is a jump in the derivative of the relaxation time with respect to the reaction rates at the boundaries. This is the dynamical phase transition. So the dynamical phase transition studied here is a discontinuity in the derivative of the relaxation time (from zero to non-zero) with respect to reaction rates in the bulk and at the boundaries. We use the method presented there, for our two-species models. Defining the two parameters \(A\), and \(B\) as

\[
A := \frac{d_1 - D'_2}{\sqrt{d_1 d_2}}, \quad B := \frac{d_2 - D'_1}{\sqrt{d_1 d_2}},
\]

it is shown in [17], depending on the phase of the system, the relaxation times of the models may be \(T_0\), \(T_A\) or \(T_B\)

\[
T_0 = \frac{1}{(\sqrt{d_1} - \sqrt{d_2})^2}, \quad T_A = \frac{d_1 - D'_2}{D'_2(d_1 - D'_2 - d_2)}, \quad T_B = \frac{d_2 - D'_1}{D'_1(d_2 - D'_1 - d_1)}.
\]

Three phases may occur:

\[
\begin{align*}
(1) & \quad A < 1, B < 1 : T_0, \\
(2) & \quad A < 1, B > 1 : T_B, \\
(3) & \quad A > 1, B < 1 : T_A.
\end{align*}
\]

The case \(A > 1, B > 1\) does not occur in any of the above mentioned models.

Let us first consider the case \(K_1\). We have

\[
A = \frac{(\omega_{42} + \omega_{43}(b_1/a_1)) - (a_2^*/a_2)}{\sqrt{(\omega_{24} + \omega_{27}(b_1/a_1))(\omega_{42} + \omega_{43}(b_1/a_1))}} \quad \text{or} \quad \frac{(\omega_{24} + \omega_{27}(b_1/a_1)) - (a_2^*/a_2)}{\sqrt{(\omega_{24} + \omega_{27}(b_1/a_1))(\omega_{42} + \omega_{43}(b_1/a_1))}}
\]

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If \((\omega_2 + \omega_3(b_1/a_1)) > (\omega_2 + \omega_3(b_1/a_1))\) one arrives at

\[
\sqrt{\left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right) \left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right)} > \left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right).
\]

(90)

So, \(\sqrt{\omega_2 + \omega_3(b_1/a_1)}(\omega_2 + \omega_3(b_1/a_1)) > (\omega_2 + \omega_3(b_1/a_1)) - (\alpha_{21}/a_2)\), which gives \(A < 1\). For

\[
\left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right) > \left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right),
\]

(91)

it can be shown that \(B\) is also less than 1. If

\[
\left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right) < \left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right),
\]

(92)

one again can show that both \(A\), and \(B\) are less than 1. Thus this model belongs to the region 1. So the model \(K_1\) possesses no dynamical phase transition, and the relaxation time is \(T_0\). \(T_0\) has no dependence on boundary rates and only depends on the reaction rates in the bulk. This result is the same as the one found for ASEP, which is a single-species model. It should be noted that this model is a generalization of ASEP. If one forgets about the difference of two particles, \(K_1\) changes to ASEP.

In the case of \(\rho_1 \neq 0, 1, \rho_2 = 0\), defining

\[
\Omega_1 := \frac{1}{(1 - \rho_1)} \left[\left(\omega_2 + \omega_3 \frac{b_1}{a_1}\right)(1 - \rho_1) + (\omega_4 + \omega_5 + \omega_6 + \omega_7 + \omega_8 + \omega_9 + \omega_{10} + \omega_{11} + \omega_{12} + \omega_{13})\right],
\]

\[
\Omega_2 := \frac{1}{\omega_2 + \omega_3 \frac{b_1}{a_1}},
\]

one arrives at

\[
A = \frac{\Omega_2 - (\alpha_{12}a_1 + \alpha_{13}b_1/\rho_1)}{\sqrt{\Omega_1 \Omega_2}},
\]

\[
B = \frac{\Omega_1 - (\alpha_{12}a_1 + \alpha_{13}b_1/\rho_1(1 - \rho_1))}{\sqrt{\Omega_1 \Omega_2}} = \frac{\Omega_2/((1 - \rho_1)) - (\alpha_{13}/b_1)}{\sqrt{\Omega_1 \Omega_2}}.
\]

(93)

if \(\Omega_1 < \Omega_2\), then \(B < 1\) and \(A\) can be smaller or greater than 1 and if \(\Omega_1 > \Omega_2\), \(A < 1\) and \(B\) can be smaller or greater than 1. So, in this case regions 1, 2 or 3 are possible. There are three distinct relaxation times. \(T_0\) is bulk dominated and depends only on reaction rates in the bulk, while \(T_A\) and \(T_B\) depend both on the reaction rates in the bulk and at the boundaries. So in this model there are three distinct phases available for the system,
and this model may experience dynamical phase transitions. Changing the reaction rates at the bulk or at the boundaries may lead to phase transitions.

Finally, in the case $\rho_1 = 1, \rho_2 = 0$, defining

$$\Omega'_1 := (\omega_{14}a_1 + \omega_{17}b_1),$$
$$\Omega'_2 := (\omega_{54} + \omega_{64} + \omega_{84} + \omega_{94})a_1 + (\omega_{57} + \omega_{67} + \omega_{87} + \omega_{97})b_1,$$

it can be shown that this model’s parameters may be in any of the regions 1, 2 or 3. So this model may also experience dynamical phase transitions. It is known that single-species models have three distinct phases [17]. Here, it is seen that the two-species models considered here are also restricted to regions 1, 2 and 3.

6. Discussion

In this work, we presented a method for classifying $n$-species particle systems possessing single-shock solutions. This classification provides a simple strategy, adopting only the occupation probabilities of particles. We applied this method to two-and then three-species systems.

We have made a detailed study on the four two-species models $K_1, K_2$, ($\rho_1 \neq 0, 1, \rho_2 = 0$) and ($\rho_1 = 1, \rho_2 = 0$). For all these models some new results have been found here. In [16] the three models $K_1$, ($\rho_1 \neq 0, 1, \rho_2 = 0$) and ($\rho_1 = 1, \rho_2 = 0$) have been studied. In this paper, with the same assumptions, more general solutions have been found. This shows there are some unnecessary constraints in [16] which could be eliminated. For example, for ($\rho_1 = 1, \rho_2 = 0$) there should be no constraints on $\omega_{22}, \omega_{23}$, because the states $\emptyset A, \emptyset B$ do not exist in the final state, and also the transition rates $\omega_{56}, \omega_{58}, \omega_{59}, \omega_{65}, \omega_{68}, \omega_{69}, \omega_{85}, \omega_{86}, \omega_{89}, \omega_{95}, \omega_{96}, \omega_{98}$ from the fifth, sixth, eighth, ninth columns of the local Hamiltonian $h$ were set equal to zero, while generally they could be non-zero (see section 4.2.2).

The model investigated in [15] resembles the model $K_2$ of this paper in some of the initial assumptions; the non-zero bulk transition rates and the condition (47) of this paper are the same. However, each paper has presented a completely distinct solution. In [15], the occupation probabilities have been assumed to be equal to 0 and 1 in one part of the lattice, which required three of the ten transition rates to be zero. This model is a particular example of the more general model $\rho_1 \neq 0, 1, \rho_2 = 0$ (section 4.2.1). We have found another solution with the assumption that the occupation probabilities should be necessarily different from 0 to 1. Consequently, one should note that the two papers presented two different models.

Moreover, the model studied in section 4.1.1 with a special choice of symmetry has been previously studied in [14]. A special example of this model when the reaction rates are eliminated has also been presented in [13]. We derived the same relations for this case in section 4.1.1.

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Appendix

The simplest forms of the boundary relations of the case $K_2$ are

\[ \begin{align*}
(1) & \quad -\alpha_2^e (1 - \rho_2) + (\alpha_{12}^f + \alpha_{32}^f) a_2 - \alpha_{23}^f b_2 + (\alpha_{31}^e (1 - \rho_2) + \alpha_{32}^e a_2 - (\alpha_{13}^e + \alpha_{23}^e) b_2) \frac{a_2 - a_1}{b_2 - b_1} = I_1 \\
(2) & \quad -\alpha_2^e (1 - \rho_2) + (\alpha_{12}^r + \alpha_{32}^r) a_2 - \alpha_{23}^r b_2 + (\alpha_{31}^e (1 - \rho_2) + \alpha_{32}^r a_2 - (\alpha_{13}^e + \alpha_{23}^r) b_2) \frac{a_2 - a_1}{b_2 - b_1} = -I_1 \\
(3) & \quad -\alpha_2^e (1 - \rho_1) + (\alpha_{12}^e + \alpha_{32}^e) a_1 - \alpha_{23}^e b_1 + (\alpha_{31}^e (1 - \rho_1) + \alpha_{32}^e a_1 - (\alpha_{13}^e + \alpha_{23}^e) b_1) \frac{a_2 - a_1}{b_2 - b_1} = I_2 \\
(4) & \quad -\alpha_2^e (1 - \rho_1) + (\alpha_{12}^r + \alpha_{32}^r) a_1 - \alpha_{23}^r b_1 + (\alpha_{31}^e (1 - \rho_1) + \alpha_{32}^r a_1 - (\alpha_{13}^e + \alpha_{23}^r) b_1) \frac{a_2 - a_1}{b_2 - b_1} = -I_2 \\
(5) & \quad \frac{1}{b_2 - b_1} (\alpha_{31}^e (1 - \rho_2) - \alpha_{32}^r a_2 + (\alpha_{13}^e + \alpha_{23}^r) b_2) = I_3 \\
(6) & \quad \frac{1}{b_2 - b_1} (\alpha_{31}^e (1 - \rho_1) + \alpha_{32}^e a_1 - (\alpha_{13}^e + \alpha_{23}^e) b_1) = I_4.
\end{align*} \]

Defining

\[ M := \left( \frac{(a_1 b_2 - a_2 b_1) (\rho_1 - \rho_2)}{(a_1 - a_2) (b_1 - b_2)} \right) \]  

(A.2)

$I_1, I_3, I_2, I_4$ become

\[ \begin{align*}
I_1 b_1 & = -I_2 b_2 \\
I_2 & = d_1 \left( a_1 b_2 - a_2 b_1 \right)^3 \frac{(\rho_1 - \rho_2)}{a_1 a_2 b_1 (a_1 - a_2) (b_1 - b_2)} \\
I_4 & = d_1 \left( 1 + M^2 \frac{(1 - 2b_1)}{a_1 (1 - \rho_1)} \right) \\
I_3 & = d_1 \left( \frac{b_2^2}{b_1^2} + M^2 \frac{(1 - 2b_2)}{a_1 (1 - \rho_1)} \right).
\end{align*} \]  

(A.3)

As can be seen, if one of the constants $d_1, I_1, I_3, I_2, I_4$ is given, the other constants will be obtained from the above mentioned relations.

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