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Uphill in Reaction-Diffusion Multi-species Interacting Particles Systems

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Abstract
We study reaction-diffusion processes with multi-species particles and hard-core interaction. We add boundary driving to the system by means of external reservoirs which inject and remove particles, thus creating stationary currents. We consider the condition that the time evolution of the average occupation evolves as the discretized version of a system of coupled diffusive equations with linear reactions. In particular, we identify a specific one-parameter family of such linear reaction-diffusion systems where the hydrodynamic limit behaviour can obtained by means of a dual process. We show that partial uphill diffusion is possible for the discrete particle systems on the lattice, whereas it is lost in the hydrodynamic limit.

Keywords Uphill diffusion · Interacting particle systems · Hydrodynamic limit · Duality · Linear reaction-diffusion systems

1 Introduction

1.1 Motivation and Description of Results

The aim of this paper is to study 'uphill diffusion' in multi-species interacting particle systems with hard-core interaction. We analyse systems consisting of n types of particles and add boundary reservoirs injecting and removing particles. Here, uphill diffusion means that mass flows from regions with lower density to regions with higher density. Uphill diffusion is thus a violation of Fick's law. This phenomenon has been reported in a single-species system in the presence of a phase transition (see [1–5] for 1D particle systems with Kac potentials and [6] for 2D lattice gases related to the Ising model). In multicomponent systems, uphill diffusion arises as a result of the competition between the gradients of each species [7–12]. The phenomenon whereby current in a stationary system is in a direction opposite to an

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external driving field has also been named ‘absolute negative mobility’ in [13]. Multi-species particle systems have been much studied in the recent literature, especially in relation to the notion of duality [14–22].

For diffusive models with a single species, transport of mass on a finite volume (here assumed to be the unit d-dimensional cube) is often described by the continuity equation

$$\frac{\partial}{\partial t}\rho = -\nabla \cdot J \tag{1}$$

and the Fick’s law

$$J = -\sigma \nabla \rho \tag{2}$$

Here $\rho : [0, 1]^d \times \mathbb{R}_+ \to [0, 1]$ is the density of mass, $J : [0, 1]^d \times \mathbb{R}_+ \to \mathbb{R}$ is the current, and $\sigma > 0$ is the diffusivity coefficient (that we assume constant throughout this paper). Equations (1) and (2) can be obtained as the hydrodynamical limit of diffusive interacting particle systems of “gradient type” [23], such as the simple symmetric exclusion process or the Kipnis-Marchioro-Presutti model [24]. Fick’s law (2) tells us that the total flow is opposite to the density gradient.

For multi-component systems with n species, considering the vectors $\boldsymbol{\rho} = (\rho^{(1)}, \ldots, \rho^{(n)})$ and $\boldsymbol{J} = (J^{(1)}, \ldots, J^{(n)})$, where $\rho^{(i)}(x, t)$ and $J^{(i)}(x, t)$ denote the density and the current of the i$^{\text{th}}$ species, the generalization of (1) and (2) is

$$\frac{\partial}{\partial t}\boldsymbol{\rho} = -\nabla \cdot \boldsymbol{J} \tag{3}$$

and

$$\boldsymbol{J} = -\boldsymbol{\Sigma} \cdot \nabla \boldsymbol{\rho}. \tag{4}$$

where $\boldsymbol{\Sigma}$ is now the $n \times n$ matrix of diffusion and ’cross-diffusion’ coefficients. When $\boldsymbol{\Sigma}$ is non-diagonal, then uphill diffusion is possible [9–11]. We distinguish between the case of *‘partial’ uphill*, which is obtained when the current of a given species has the same sign of the boundary density gradient of that species, and *‘global’ uphill*, which arises when the total mass flows from a region of lower total density to a region of higher total density (see Sect. 1.2 for definitions of partial and global uphill).

In this paper, we shall investigate partial uphill diffusion for hard-core multi-species interacting particle systems. Our analysis will have two targets: on one hand, we would like to understand conditions on the rates defining the microscopic dynamics so that the system is described by a linear reaction-diffusion system on a regular lattice; on the other hand, we aim to understand if and how such particle systems display partial uphill diffusion in the large scale limit. To achieve those targets we will consider the *average occupation* of each species, which is a proxy for the true density. In the spirit of [25] and [26] we shall impose that the equations for the average occupation of the species are closed. Furthermore, we shall require that the evolution of the average occupation is described by the a discretized version of (3) and (4). Actually, besides diffusion, we shall further include the possibility of reaction terms, as described in the next subsection. Our main results can be summarized as follows:

- We show that the request of a linear reaction-diffusion system on a regular lattice imposes constraints on the values of the “diffusivity matrix” and the reaction coefficient (see Theorem 4.1).
- We identify a specific multi-species interacting particle system (see again Theorem 4.1) for which the closure of correlation functions is accompanied by duality (see Sect. 5). To our knowledge, this is the first multi-species interacting particle system with reaction *and* diffusion for which one can prove the existence of a dual process (see [23] for

a perturbative treatment of reaction-diffusion in the presence of duality for the sole diffusive dynamics).

- Duality then leads to the proof of the hydrodynamic limit with the standard correlation functions method [23]. Surprisingly, we shall see that – although the microscopic dynamics has non-zero 'cross-diffusivity' terms – macroscopically the empirical mass distribution of each species satisfies hydrodynamic PDE's where the species are coupled only by the reaction term. In other words, after a suitable space/time diffusive scaling, the diffusivity matrix is necessarily diagonal and therefore partial uphill is absent. This is consistent with [27, 28] where it has been observed that the densities of eq. (3) and (4) remain positive if and only if the cross diffusivity terms are null.

We conclude this introduction with a discussion about uphill diffusion for Eqs. (3) and (4) plus a linear reaction term.

1.2 Steady State Uphill Diffusion in Multi-component Systems

In this work we restrict ourselves to the case of two species diffusing on the unit interval. In the case of a larger number of species one may expect that more complex regions of uphill diffusion can arise. Let us call $\rho^{(\alpha)}(x,t) : [0,1] \times [0,\infty) \to [0,1]$ the density of the species $\alpha \in \{0,1,2\}$. We impose the constraint $\rho^{(0)} + \rho^{(1)} + \rho^{(2)} = 1$, which will represent later the hard-core interaction of the associated interacting particle system. It is then enough to study the evolution of $\rho^{(1)}$ and $\rho^{(2)}$, which will be assumed to be smooth functions. We consider a Cauchy problem with Dirichlet boundary conditions, where each density is endowed with an initial datum $\rho^{(\alpha)}(x,0) = \rho_0^{(\alpha)}(x)$ and boundary conditions $\rho^{(\alpha)}(0,t) = \rho_L^{(\alpha)}$ and $\rho^{(\alpha)}(1,t) = \rho_R^{(\alpha)}$ for $\alpha = 1, 2$. We are interested in the stationary properties. We consider

$$\begin{aligned} \partial_t \rho^{(1)} &= \sigma_{11} \partial_x^2 \rho^{(1)} + \sigma_{12} \partial_x^2 \rho^{(2)} + \Upsilon \left(\rho^{(2)} - \rho^{(1)} \right) \\ \partial_t \rho^{(2)} &= \sigma_{21} \partial_x^2 \rho^{(1)} + \sigma_{22} \partial_x^2 \rho^{(2)} + \Upsilon \left(\rho^{(1)} - \rho^{(2)} \right) \end{aligned} \tag{5}$$

where the matrix

$$\Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \tag{6}$$

is assumed to have positive determinant and the sum of all its elements to be positive (the reason for this assumption will become clear in what follows, see below Eq. (10)). The stationary diffusive currents are given by

$$\begin{aligned} J^{(1)}(x) &= -\sigma_{11} \partial_x \rho^{(1)}(x) - \sigma_{12} \partial_x \rho^{(2)}(x) \\ J^{(2)}(x) &= -\sigma_{21} \partial_x \rho^{(1)}(x) - \sigma_{22} \partial_x \rho^{(2)}(x) \end{aligned} \tag{7}$$

We distinguish two cases:

- *global uphill*: this happens when the boundary values of the total boundary density $\rho_L = \rho_L^{(1)} + \rho_L^{(2)}$ and $\rho_R = \rho_R^{(1)} + \rho_R^{(2)}$ and the total current $J(x) = J^{(1)}(x) + J^{(2)}(x)$ are such that either $\rho_L < \rho_R$ and $J(x) > 0 \ \forall x \in [0,1]$, or $\rho_L > \rho_R$ and $J(x) < 0$ $\forall x \in [0,1]$.
- *partial uphill for the* i^{th} *species*: for boundary values $\rho_L^{(1)}, \rho_L^{(2)}, \rho_R^{(1)}, \rho_R^{(2)} \geq 0$, the system has stationary partial uphill diffusion for the species $i \in \{1,2\}$ if $\rho_L^{(i)} < \rho_R^{(i)}$ and $J^{(i)}(x) > 0 \ \forall x \in [0,1]$, or if $\rho_L^{(i)} > \rho_R^{(i)}$ and $J^{(i)}(x) < 0 \ \forall x \in [0,1]$.

Clearly, in the case where each density simply obeys a one dimensional heat equation

$$\begin{aligned}\partial_t \rho^{(1)}(x,t) &= \sigma_{11}\partial_x^2 \rho^{(1)}(x,t)\\ \partial_t \rho^{(2)}(x,t) &= \sigma_{22}\partial_x^2 \rho^{(2)}(x,t)\end{aligned} \tag{8}$$

no uphill diffusion (neither global nor partial) is possible.

Global uphill diffusion can be obtained by keeping the matrix Σ diagonal and adding a reaction term, i.e.

$$\begin{aligned}\partial_t \rho^{(1)} &= \sigma_{11}\partial_x^2 \rho^{(1)} + \Upsilon\left(\rho^{(2)} - \rho^{(1)}\right)\\ \partial_t \rho^{(2)} &= \sigma_{22}\partial_x^2 \rho^{(2)} + \Upsilon\left(\rho^{(1)} - \rho^{(2)}\right)\end{aligned} \tag{9}$$

In [12] the above equations have been obtained as the hydrodynamical limit of a switching interacting particle system, and the region with global uphill has been explicitly characterized.

To obtain partial uphill diffusion one needs to consider the more general case (5) with a *non-diagonal* matrix Σ. We give the stationary solution of (5) from which the existence of partial uphill can be obtained. The computations to obtain these profiles are reported in Appendix A. Introducing the constants $A = \Upsilon\frac{\sigma_{12}+\sigma_{22}}{\sigma_{11}\sigma_{22}-\sigma_{12}\sigma_{21}} > 0$ and $B = -\Upsilon\frac{\sigma_{11}+\sigma_{21}}{\sigma_{11}\sigma_{22}-\sigma_{12}\sigma_{21}} < 0$, the steady state density profiles reads

$$\begin{aligned}\rho^{(1)}(x) &= E + Fx + C\left(1+\frac{A-B}{B}\right)e^{-\sqrt{A-B}x} + D\left(1+\frac{A-B}{B}\right)e^{\sqrt{A-B}x}\\ \rho^{(2)}(x) &= E + Fx + Ce^{-\sqrt{A-B}x} + De^{\sqrt{A-B}x}\end{aligned} \tag{10}$$

where the constants C, D, E, F are determined by the boundary conditions as follows:

$$E = \frac{A\,\rho_L^{(2)} - B\,\rho_L^{(1)}}{A-B} \quad C = \frac{B\left(\rho_L^{(1)}e^{2\sqrt{A-B}} - \rho_L^{(2)}e^{2\sqrt{A-B}} - \rho_R^{(1)}e^{\sqrt{A-B}} + \rho_R^{(2)}e^{\sqrt{A-B}}\right)}{(A-B)\left(e^{2\sqrt{A-B}}-1\right)}$$

$$F = -\frac{A\,\rho_L^{(2)} - A\,\rho_R^{(2)} - B\,\rho_L^{(1)} + B\,\rho_R^{(1)}}{A-B} \quad D = \frac{B\left(\rho_L^{(1)} - \rho_L^{(2)} - \rho_R^{(1)}e^{\sqrt{A-B}} + \rho_R^{(2)}e^{\sqrt{A-B}}\right)}{A-B-A\,e^{2\sqrt{A-B}} + B\,e^{2\sqrt{A-B}}}$$

From Eq. (10) we see that the conditions $\sigma_{11}+\sigma_{12}+\sigma_{21}+\sigma_{22} > 0$ and $\sigma_{11}\sigma_{22}-\sigma_{12}\sigma_{21} > 0$ guarantees $A-B > 0$, i.e., non-oscillating solutions. Here we plot in Fig. 1 the stationary densities and currents for a specific choice of the boundary values and of the diffusivity matrix and reaction term. From the picture one can clearly see partial uphill diffusion (in the absence of global uphill).

1.3 Organization of the Paper

Our paper is organized as follows. In Sect. 2 we describe the generic form of a multi-species Markov process with constant rates allowing at most one particle per site. We define the process on a spatial structure given by a graph G and we compare to other models that have been studied in the literature. We then compute in Sect. 3 the evolution equation for the average occupation variables of each species.

From Sect. 4 onward we specialize to the case of *two species on one-dimensional chains*. We start, in Sect. 4, by imposing that the average occupations evolve as the discretized version of (5). This leads to a linear algebraic system, which can be solved. As a result, sufficient and necessary conditions on the diffusivity matrix Σ and the reaction coefficient Υ in order to

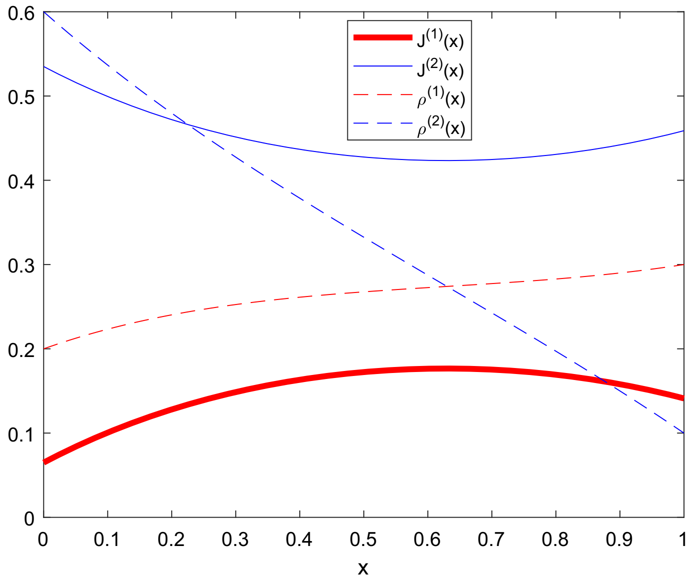

Fig. 1 Density profile (dashed lines) and currents (continuous line). The red color is for species 1 and the blue color for species 2. The boundary values are $(\rho_L^{(1)}, \rho_L^{(2)}, \rho_R^{(1)}, \rho_R^{(2)}) = (0.2, 0.6, 0.3, 0.1)$. The diffusivity matrix and the reaction term are $\sigma_{11} = \sigma_{22} = \Upsilon = 1$ and $\sigma_{12} = \sigma_{21} = 1/2$

have the discrete version of a linear reaction-diffusion system are identified in Theorem 4.1. Furthermore, it is shown in the same theorem an explicit example of a one-parameter family of symmetric processes having such linear and discrete reaction-diffusion structure. This specific model is further analyzed in Sect. 5, where we prove duality and the hydrodynamic limit. Section 6 draws the conclusions of our analysis.

2 Hard-Core Multi-species Particles on a Graph G = (V, E)

Notation: In what follows, we use greek letters $(\alpha, \beta, \gamma, \delta, \ldots)$ to denote the species of the particles and latin letters $(x, y, z, \ldots)$ to denote the sites of the graph.

In this section we define our microscopic model on a generic graph $G = (V, E)$. Here, the set $V = \{1, 2, \ldots, N\}$ is a collection of N vertices. The set of edges E is such that the graph is connected, oriented (directed) and without self-edges. On this graph G we consider a system of interacting particles, each of which has its own type/species. We assume there are n species. Furthermore, on each vertex of the graph there is at most one particle (hard-core exclusion rule). Thus, the occupation variable at each vertex takes values in $\{0, 1, 2, \ldots n\}$, with type 0 denoting the empty site.

The dynamical rule is due to a one-body interaction and a two-body interaction:

- on each site $x \in V$ the occupation of type γ changes to type α at rate $a_x W_\gamma^\alpha(x)$;
- on each edge $(x, y) \in E$ the occupations of type (γ, δ) changes to type (α, β) at rate $a_{x,y}\Gamma_{\gamma\delta}^{\alpha\beta}$.

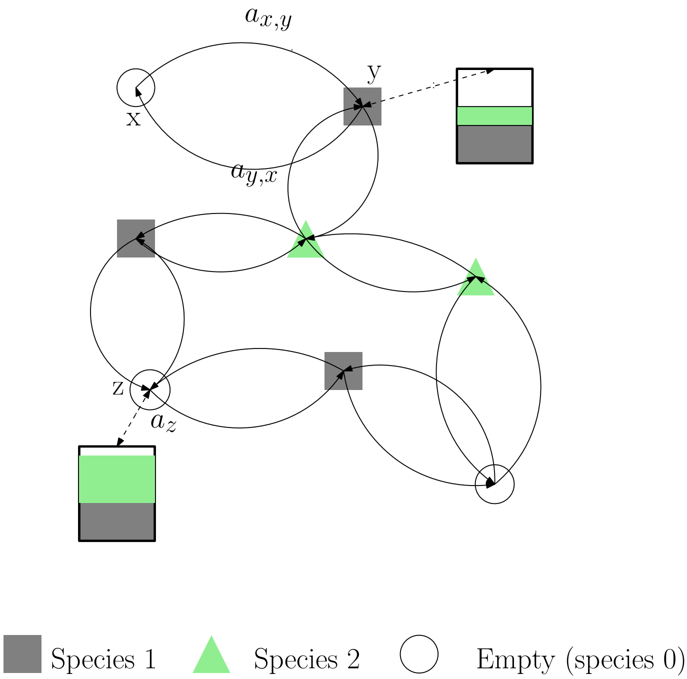

Fig. 2 Hard-core two-species particles on a graph with 8 vertices and 2 reservoirs. Grey squares identify the species 1, green triangles the species 2, and white circles the empty state. The reservoirs are represented by rectangles, where the interior colours denote the density of species

Here the non-negative numbers $\{a_{x,y}\}_{(x,y)\in E}$ and $\{a_x\}_{x\in V}$ are, respectively, edge weights (conductances) and site weights (local inhomogeneities) of the graph. For a visual representation of the process with two species see Fig. 2.

2.1 Process Definition

On the graph $G = (V, E)$, we consider the Markov process $\{\eta(t); t \geq 0\}$ with state space $\Omega = \{0, 1, 2, \ldots, n\}^V$. A configuration of the process is denoted by $\eta = (\eta_x)_{x\in V}$, where each component can take the values $\eta_x \in \{0, 1, ..., n\}$ and where $\eta_x = \alpha$ means the presence of the species α at the site x. We recall that $\eta_x = 0$ is interpreted as an empty site.

The process is defined by the generator $\mathcal{L}$ working on functions $f : \Omega \to \mathbb{R}$ as

$$(\mathcal{L}f)(\eta) = (\mathcal{L}_{edge}f)(\eta) + (\mathcal{L}_{site}f)(\eta), \tag{11}$$

where

$$(\mathcal{L}_{edge}f)(\eta) = \sum_{(x,y)\in E} a_{x,y} \cdot (\mathcal{L}_{x,y}f)(\eta)$$

and

$$(\mathcal{L}_{site}f)(\eta) = \sum_{x\in V} a_x \cdot (\mathcal{L}_x f)(\eta)$$

We shall explain the two generators $\mathcal{L}_{edge}$ and $\mathcal{L}_{site}$ in the following subsections.

2.1.1 The Edge Generator

We introduce the $(n+1)^2 \times (n+1)^2$ matrix Γ whose elements are rates of transition for the particle jumps on each edge. More precisely, we denote by $\Gamma_{\gamma\delta}^{\alpha\beta}$ the rate to change the configuration η with $\eta_x = \gamma, \eta_y = \delta$ to the configuration η' with $\eta'_x = \alpha, \eta'_y = \beta$, while $\eta'_z = \eta_z$ for all $z \neq x, y$. Thus, the single-edge generator is given by

$$\begin{aligned} &\mathcal{L}_{x,y} f(\eta_1, \ldots, \gamma, \ldots, \delta, \ldots, \eta_N) \\ &\quad = \sum_{\alpha,\beta=0}^{n} \Gamma_{\gamma\delta}^{\alpha\beta} \left[f(\eta_1, \ldots, \alpha, \ldots, \beta, \ldots, \eta_N) - f(\eta_1, \ldots, \gamma, \ldots, \delta, \ldots, \eta_N) \right] \end{aligned} \quad (12)$$

where

$$\begin{aligned} \Gamma_{\gamma\delta}^{\alpha\beta} &\geq 0 \quad \text{if} \quad (\alpha, \beta) \neq (\gamma, \delta) \\ \sum_{(\gamma,\delta)\in\{0,1,2,\ldots,n\}^2 \,:\, (\gamma\delta)\neq(\alpha,\beta)} \Gamma_{\gamma\delta}^{\alpha\beta} &= -\Gamma_{\alpha\beta}^{\alpha\beta} \quad \forall (\alpha, \beta) \in \{0, 1, 2, \ldots, n\}^2 . \end{aligned}$$

2.1.2 The Site Generator

Having in mind that the site generator will describe a 'boundary' driving leading the system to a non-equilibrium steady state, we assume that on each site there is a process which injects and removes particles at a rate which is space-dependent. Thus, for each vertex $x \in V$, we introduce the $(n+1) \times (n+1)$ matrix $W(x)$ whose elements are rates of transitions on that vertex. More precisely, we denote by $W_\gamma^\alpha(x)$ the rate to change the configuration η with $\eta_x = \gamma$ into the configuration η' with $\eta'_x = \alpha$, while $\eta'_z = \eta_z$ for all $z \neq x$. The single-vertex generator is given by

$$\begin{aligned} &\mathcal{L}_x f(\eta_1, \ldots, \gamma, \ldots, \eta_N) \\ &\quad = \sum_{\alpha=0}^{n} W_\gamma^\alpha(x) \left[f(\eta_1, \ldots, \alpha, \ldots., \eta_N) - f(\eta_1, \ldots, \gamma, \ldots, \eta_N) \right] \end{aligned} \quad (13)$$

where

$$\begin{aligned} W_\gamma^\alpha(x) &\geq 0 \quad \text{if} \quad \alpha \neq \gamma \\ \sum_{\gamma\in\{0,1,2,\ldots,n\}:\gamma\neq\alpha} W_\gamma^\alpha(x) &= -W_\alpha^\alpha(x) \quad \forall \alpha \in \{0, 1, 2, \ldots, n\} . \end{aligned}$$

2.2 Comparison to Other Processes

Here, we discuss the relation of the general dynamics described above to some multi-species processes considered in the past literature (we consider here the case of homogeneous conductances and inhomogeneities $a_{x,y} = a_x = 1$). We shall mostly limit the discussion to *symmetric* systems (for asymmetric models there is also a large literature, see for instance [14] and references therein). In most cases, previous analyses have been restricted to a regular lattice or a one-dimensional chain.

- *General multi-species models*. The edge dynamics of the reaction-diffusion particle system in Sect. 2.1 has been considered on a d-dimensional lattice in [25] for the case $n = 1$

species and in [26] for the case of an arbitrary number of species. In those papers, sufficient conditions on the rates $\Gamma^{\alpha\beta}_{\gamma\delta}$ to guarantee the existence of dual process have been identified.

- *Multi-species exclusion processes*. The edge dynamics of multi-species simple symmetric exclusion process (SSEP) on a d-dimensional lattice, with at most one-particle per site, has been considered in [29]. It corresponds to the model of Sect. 2.1 with $\Gamma^{\alpha 0}_{0\alpha} = \Gamma^{0\alpha}_{\alpha 0} \neq 0$ for all $\alpha = 0, 1, \dots, n$, while all other off-diagonal elements of the matrix Γ vanish, as well as the elements of the matrices $W(x)$. For this model, the hierarchy of equations for the correlations does not close, and the hydrodynamic limit has been shown in [29] to be given by two coupled *non-linear* heat equations. An open boundary version of the model with simple symmetric exclusion dynamic in the bulk has been presented in [7]. It corresponds to the model of Sect. 2.1 with $\Gamma^{0b}_{b0} = \Gamma^{b0}_{0b} = D_b$ and with boundary rates $W^b_0(1) = \alpha_b$, $W^0_b = \gamma_b$, $W^b_0(N) = \beta_b$, $W^0_b(N) = \delta_b$ (here b labels the species). All the other off-diagonal elements Γ and $W(z)$ vanish.
- *Multi-species stirring process*. In the stirring process [30, 31], every couple of types is exchanged in position with the same rate, which can be taken equal to 1 without loss of generality. Thus, the bulk dynamics of the stirring process corresponds to the case $\Gamma^{\delta\gamma}_{\gamma\delta} = 1$ for all $\gamma, \delta = 0, 1, \dots, n$, while all other off-diagonal elements of the matrix Γ vanish. The hydrodynamic limit of the stirring process on a lattice is given by n independent diffusions, i.e. the generalization of (8) to n types. The multi-species stirring process on a chain with boundary driving has been studied in [32] with the choice $W^b_\gamma(1) = \alpha_b$ and $W^b_\gamma(N) = \beta_b$. With this particular choice of the boundary rates the model is solvable and correlation functions in the non equilibrium steady state have been computed using the matrix product ansatz.
- *Multi-species switching process*: A different set-up for multi-species particle systems has been recently proposed in [12, 33]. One considers n "piled" copies of the graph G, each with its own single-type dynamics. The possibility of changing type is described by a *switching rate* between layers. This set-up eliminates the constraint of one particle per site, in the sense that the projection of the dynamics on the columns of the piled graph allows the presence of several particle of different types on the same "base" site. In the case where each layer is a one-dimensional chain and two-layers are considered, the hydrodynamic limit has been shown to be given by the "weakly" coupled reaction diffusion equation (9). When boundary reservoirs are added, global uphill diffusion and boundary layers are possible [12].

3 Evolution Equations for the Average Occupation

For the model introduced in Sect. 2.1, we define the average of the occupation variable of each species $\zeta \in \{0, 1, \dots, n\}$ at time $t \geq 0$ and at the vertex $z \in V$

$$\mu^{(\zeta)}_z(t) = \mathbb{E}\left[\mathbb{1}_{\{\mathcal{I}^\zeta_z\}}(\eta(t))\right]. \tag{14}$$

Similarly, we consider the time-dependent correlations (multiple occupancy variables) between species $\zeta, \zeta' \in \{0, 1, \dots, n\}$ at points $z, z' \in V$

$$c^{(\zeta,\zeta')}_{z,z'}(t) = \mathbb{E}\left[\mathbb{1}_{\{\mathcal{I}^\zeta_z\}}(\eta(t))\mathbb{1}_{\{\mathcal{I}^{\zeta'}_{z'}\}}(\eta(t))\right]. \tag{15}$$

Here $\mathcal{I}_z^\zeta = \{\eta \in \Omega : \eta_z = \zeta\}$ and $\mathbb{1}_{\mathcal{I}}$ denotes the indicator function of the set $\mathcal{I}$. The notation $\mathbb{E}[f(\eta(t))] = \int \nu_0(d\eta)\mathbb{E}_\eta [f(\eta(t))]$ denotes the expectation in the process $\{\eta(t)\}_{t\geq 0}$ started from the initial measure ν_0. The evolution equation of the density of the ζ-species can be obtained by acting with the generator. We have

$$\frac{d\mathbb{E}\left[\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}(\eta(t))\right]}{dt} = \mathbb{E}\left[\left(\mathcal{L}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta(t))\right]. \tag{16}$$

In the following section we evaluate the right hand side of this equation by considering first edge contributions and then site contributions.

3.1 Action of $\mathcal{L}_{x,y}$

If $z \notin \{x, y\}$ then obviously $\left(\mathcal{L}_{x,y}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = 0$. Otherwise, recalling that the graph G is directed and the notation of [26], we have the following: when we fix $z = x$ then

$$\left(\mathcal{L}_{z,y}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = A_1^\zeta + \sum_{\delta=1}^n F_{+1}^{\zeta\delta}\mathbb{1}_{\{\mathcal{I}_y^\delta\}}(\eta) + \sum_{\gamma=1}^n B_1^{\zeta\gamma}\mathbb{1}_{\{\mathcal{I}_z^\gamma\}}(\eta) + \sum_{\gamma,\delta=1}^n G_{+1}^{\zeta\gamma\delta}\mathbb{1}_{\{\mathcal{I}_y^\gamma\}}(\eta)\mathbb{1}_{\{\mathcal{I}_z^\delta\}}(\eta) \tag{17}$$

and when we fix $z = y$ then

$$\left(\mathcal{L}_{x,z}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = A_2^\zeta + \sum_{\gamma=1}^n F_{-1}^{\zeta\gamma}\mathbb{1}_{\{\mathcal{I}_x^\gamma\}}(\eta) + \sum_{\delta=1}^n C_2^{\zeta\delta}\mathbb{1}_{\{\mathcal{I}_z^\delta\}}(\eta) + \sum_{\gamma,\delta=1}^n G_{-1}^{\zeta\gamma\delta}\mathbb{1}_{\{\mathcal{I}_z^\gamma\}}(\eta)\mathbb{1}_{\{\mathcal{I}_x^\delta\}}(\eta) \tag{18}$$

where the constants are defined as follows:

1. *zero-order terms*:

$$A_1^\zeta = \sum_{\beta=0}^n \Gamma_{00}^{\zeta\beta} \qquad A_2^\zeta = \sum_{\beta=0}^n \Gamma_{00}^{\beta\zeta}$$

2. *first-order terms*:

$$B_1^{\zeta\gamma} = \begin{cases} \sum_{\beta=0}^n (\Gamma_{\gamma 0}^{\zeta\beta} - \Gamma_{00}^{\zeta\beta}) & \text{if } \zeta \neq \gamma \\ -\sum_{\beta=0}^n \left(\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^n \Gamma_{\zeta 0}^{\zeta'\beta} + \Gamma_{00}^{\zeta\beta}\right) & \text{if } \zeta = \gamma \end{cases}$$

$$C_2^{\zeta\delta} = \begin{cases} \sum_{\beta=0}^n (\Gamma_{0\delta}^{\beta\zeta} - \Gamma_{00}^{\beta\zeta}) & \text{if } \zeta \neq \delta \\ -\sum_{\beta=0}^n \left(\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^n \Gamma_{0\zeta}^{\beta\zeta'} + \Gamma_{00}^{\beta\zeta}\right) & \text{if } \zeta = \delta \end{cases}$$

$$F_{-1}^{\zeta\gamma} = B_2^{\zeta\gamma} = \sum_{\beta=0}^n (\Gamma_{\gamma 0}^{\beta\zeta} - \Gamma_{00}^{\beta\zeta})$$

$$F_{+1}^{\zeta\delta} = C_1^{\zeta\delta} = \sum_{\beta=0}^n (\Gamma_{0\delta}^{\zeta\beta} - \Gamma_{00}^{\zeta\beta})$$

3. *second-order terms:*

$$G_{+1}^{\zeta\gamma\delta} = D_1^{\zeta,\gamma,\delta} = \begin{cases} \sum_{\beta=0}^n (\Gamma_{\gamma\delta}^{\zeta\beta} - \Gamma_{\gamma 0}^{\zeta\beta} - \Gamma_{0\delta}^{\zeta\beta} + \Gamma_{00}^{\zeta\beta}); & \text{if } \zeta \neq \gamma \\ -\sum_{\beta=0}^n \left(\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^n \Gamma_{\zeta\delta}^{\zeta'\beta} + \Gamma_{0\delta}^{\zeta\beta}\right) + \sum_{\beta=0}^n \left(\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^n \Gamma_{\zeta 0}^{\zeta'\beta} + \Gamma_{00}^{\zeta\beta}\right) & \text{if } \zeta = \gamma \end{cases}$$

$$G_{-1}^{\zeta\gamma\delta} = D_2^{\zeta,\gamma,\delta} = \begin{cases} \sum_{\beta=0}^{n}(\Gamma_{\gamma\delta}^{\beta\zeta} - \Gamma_{\gamma 0}^{\beta\zeta} - \Gamma_{0\delta}^{\beta\zeta} + \Gamma_{00}^{\beta\zeta}) & \text{if } \zeta \neq \delta \\ -\sum_{\beta=0}^{n}\left(\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^{n} \Gamma_{\gamma\zeta}^{\beta\zeta'} + \Gamma_{\gamma 0}^{\beta\zeta}\right) + \sum_{\beta=0}^{n}\left(\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^{n} \Gamma_{0\zeta}^{\beta\zeta'} + \Gamma_{00}^{\beta\zeta}\right) & \text{if } \zeta = \delta \end{cases}$$

3.2 Action of $\mathcal{L}_x$

If $z \neq x$ then obviously $\left(\mathcal{L}_x \mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = 0$. Otherwise

$$\left(\mathcal{L}_z \mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = A^\zeta(z) + \sum_{\beta=1}^{n} F^{\zeta\beta}(z)\mathbb{1}_{\{\mathcal{I}_z^\beta\}}(\eta) \tag{19}$$

where now the constants are defined as:

1. *zero-order term*:

$$A^\zeta(z) = W_0^\zeta(z)$$

2. *first-order term*:

$$F^{\zeta\beta}(z) = \begin{cases} W_\beta^\zeta(z) - W_0^\zeta(z) & \text{if } \zeta \neq \beta \\ -\sum_{\zeta'=0\,:\,\zeta'\neq\zeta}^{n} W_\zeta^{\zeta'}(z) - W_0^\zeta(z) & \text{if } \zeta = \beta \end{cases}.$$

3.3 Action of $\mathcal{L}$

We now collect the results of the previous sections. We may write

$$\begin{aligned} \left(\mathcal{L}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) &= \sum_{x,y\,:\,(x,y)\in E} a_{x,y}\left(\mathcal{L}_{x,y}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) + \sum_x a_x\left(\mathcal{L}_x\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) \\ &= \sum_{y\,:\,(z,y)\in E} a_{z,y}\left(\mathcal{L}_{z,y}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) + \sum_{x\,:\,(x,z)\in E} a_{x,z}\left(\mathcal{L}_{x,z}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) \\ &\quad + a_z\left(\mathcal{L}_z\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta). \end{aligned}$$

Substituting (17), (18), (19) in the above expression we obtain

$$\begin{aligned} \left(\mathcal{L}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = \sum_{y\,:\,(z,y)\in E} a_{z,y} &\left(A_1^\zeta + \sum_{\delta=1}^{n} F_{+1}^{\zeta\delta}\mathbb{1}_{\{\mathcal{I}_y^\delta\}}(\eta) + \sum_{\gamma=1}^{n} B_1^{\zeta\gamma}\mathbb{1}_{\{\mathcal{I}_z^\gamma\}}(\eta) \right. \\ &\left. + \sum_{\gamma,\delta=1}^{n} G_{+1}^{\zeta\gamma\delta}\mathbb{1}_{\{\mathcal{I}_y^\gamma\}}(\eta)\mathbb{1}_{\{\mathcal{I}_z^\delta\}}(\eta) \right) \\ + \sum_{x\,:\,(x,z)\in E} a_{x,z} &\left(A_2^\zeta + \sum_{\gamma=1}^{n} F_{-1}^{\zeta\gamma}\mathbb{1}_{\{\mathcal{I}_x^\gamma\}}(\eta) + \sum_{\delta=1}^{n} C_2^{\zeta\delta}\mathbb{1}_{\{\mathcal{I}_z^\delta\}}(\eta) \right. \\ &\left. + \sum_{\gamma,\delta=1}^{n} G_{-1}^{\zeta\gamma\delta}\mathbb{1}_{\{\mathcal{I}_z^\gamma\}}(\eta)\mathbb{1}_{\{\mathcal{I}_x^\delta\}}(\eta) \right) \end{aligned}$$

$$+a_z \left(A^\zeta(z) + \sum_{\beta=1}^{n} F^{\zeta\beta}(z) \mathbb{1}_{\{\mathcal{I}_z^\beta\}}(\eta) \right). \tag{20}$$

3.4 Evolution Equations

Using Eq. (20) for the right hand side of (16) we obtain the evolution equation for the average occupation. Recalling the notation in (14) and (15) (for the sake of space we do not write the explicit t-dependence) we arrive to

$$\begin{aligned} \frac{d}{dt}\mu_z^{(\zeta)} = & \sum_{y\,:\,(z,y)\in E} a_{z,y} \left(A_1^\zeta + \sum_{\delta=1}^{n} F_{+1}^{\zeta\delta}\, \mu_y^{(\delta)} + \sum_{\gamma=1}^{n} B_1^{\zeta\gamma}\, \mu_z^{(\gamma)} + \sum_{\gamma,\delta=1}^{n} G_{+1}^{\zeta\gamma\delta}\, c_{y,z}^{(\gamma,\delta)} \right) \\ & + \sum_{x\,:\,(x,z)\in E} a_{x,z} \left(A_2^\zeta + \sum_{\gamma=1}^{n} F_{-1}^{\zeta\gamma}\, \mu_x^{(\gamma)} + \sum_{\delta=1}^{n} C_2^{\zeta\delta}\, \mu_z^{(\delta)} + \sum_{\gamma,\delta=1}^{n} G_{-1}^{\zeta\gamma\delta}\, c_{z,x}^{(\gamma,\delta)} \right) \\ & + a_z \left(A^\zeta(z) + \sum_{\beta=1}^{n} F^{\zeta\beta}(z)\, \mu_z^{(\beta)} \right). \end{aligned} \tag{21}$$

We notice that the equations for the time-dependent averages $\mu_z^{(\zeta)}(t)$ are not closed, as they involve the correlations $c_{z,z'}^{(\zeta,\zeta')}(t)$.

Remark 3.1 (The process on the lattice) The generator (11) is an generalization of the lattice generator studied in [26] to a general graph with the addition of open boundaries. Indeed, take as a special graph the d-dimensional regular lattice $\mathbb{Z}^d$ and ignore the boundaries. Then, calling $e^{(k)}$ the unit vector in the k^{th} direction ($k = 1, \ldots, d$) and defining

$$\begin{aligned} E^\zeta &= A_1^\zeta + A_2^\zeta \\ F_0^{\zeta\beta} &= C_2^{\zeta\beta} + B_1^{\zeta\beta} \end{aligned} \tag{22}$$

Equation (20) becomes

$$\left(\mathcal{L}\mathbb{1}_{\{\mathcal{I}_z^\zeta\}}\right)(\eta) = \sum_{k=1}^{d} \left\{ E^\zeta + \sum_{\beta=1}^{n} \sum_{j=-1}^{+1} F_j^{\zeta\beta} \mathbb{1}_{\{\mathcal{I}^\beta_{z+je^{(k)}}\}}(\eta) + \sum_{\beta,\beta'=1}^{n} \sum_{j=\pm1} G_j^{\zeta\beta\beta'} \mathbb{1}_{\{\mathcal{I}^\beta_{z+je^{(k)}}\}}(\eta) \mathbb{1}_{\{\mathcal{I}_z^{\beta'}\}}(\eta) \right\} \tag{23}$$

which is equation (3.12) in [26].

4 Boundary-Driven Chains with Linear Reaction-Diffusion

In this and the following sections we specialize to the case with only two species, labelled by 1 and 2. Furthermore, we specialize to the one-dimensional geometry by considering an undirected linear chain.

More precisely, the graph has N vertices labelled by $\{1, 2, \ldots, N\}$ with a distinguish role of the sites $\{1, N\}$which model two reservoirs. The interaction is of nearest neighbor type, i.e.

$$a_{x,y} = \begin{cases} 1 & \text{if} \quad |x-y| = 1 \\ 0 & \text{otherwise} \end{cases} \qquad\qquad a_x = \begin{cases} 1 & \text{if} \quad x \in \{1, N\} \\ 0 & \text{otherwise} \end{cases}$$

It is convenient to call the sites $\{2,\dots,N-1\}$ as "bulk" and the two end sites $\{1,N\}$ as "boundary". The generator of the process thus reads:

$$\mathcal{L} = \mathcal{L}_1 + \sum_{z=1}^{N-1} \mathcal{L}_{z,z+1} + \mathcal{L}_N \tag{24}$$

We specialize the result of Eq. (21) to the boundary-driven chain. Introducing $\forall\zeta,\beta=1,2$:

$$\begin{aligned} F_0^{\zeta\beta} &= B_1^{\zeta\beta} + C_2^{\zeta\beta} & E^{\zeta} &= A_1^{\zeta} + A_2^{\zeta} \\ A_L^{\zeta} &= A^{\zeta}(1) & A_R^{\zeta} &= A^{\zeta}(N) \\ F_L^{\zeta\beta} &= F^{\zeta\beta}(1) & F_R^{\zeta\beta} &= F^{\zeta\beta}(N) \end{aligned}$$

the evolution equations for the densities of the two species at site $z\in\{1,2,\dots,N\}$ are given by:

$$\frac{d}{dt}\mu_1^{(\zeta)} = A_L^{\zeta} + A_1^{\zeta} + \sum_{\beta=1}^{2}\left(\left(B_1^{\zeta\beta} + F_L^{\zeta\beta}\right)\mu_1^{(\beta)} + F_{+1}^{\zeta\beta}\mu_2^{(\beta)}\right) + \sum_{\beta,\beta'=1}^{2} G_{+1}^{\zeta\beta\beta'} c_{1,2}^{(\beta,\beta'))} \tag{25}$$

$$\frac{d}{dt}\mu_z^{(\zeta)} = E^{\zeta} + \sum_{\beta=1}^{2}\left(F_{-1}^{\zeta\beta}\mu_{z-1}^{(\beta)} + F_0^{\zeta\beta}\mu_z^{(\beta)} + F_{+1}^{\zeta\beta}\mu_{z+1}^{(\beta)}\right) + \sum_{\beta,\beta'=1}^{2}\left(G_{-1}^{\zeta\beta\beta'} c_{z-1,z}^{(\beta,\beta')} + G_{+1}^{\zeta\beta\beta'} c_{z,z+1}^{(\beta,\beta')}\right) \qquad \text{if } z\in\{2,\dots,N-1\} \tag{26}$$

$$\frac{d}{dt}\mu_N^{(\zeta)} = A_R^{\zeta} + A_2^{\zeta} + \sum_{\beta=1}^{2}\left(\left(C_2^{\zeta\beta} + F_R^{\zeta\beta}\right)\mu_N^{(\beta)} + F_{-1}^{\zeta\beta}\mu_{N-1}^{(\beta)}\right) + \sum_{\beta,\beta'=1}^{2} G_{-1}^{\zeta\beta\beta'} c_{N-1,N}^{(\beta,\beta')} \tag{27}$$

In the next section, we simplify the evolution equations for the average density by selecting a subclass of processes with closed equations and a linear structure.

4.1 Imposing the Matching

One could go further and compute the hierarchy of equations for higher-order correlation function [26]. For general choices of the rate matrices Γ and W, the equations do not close. In the following, we shall focus on those choices of rates that satisfy the following two requirements:

1. *Closure of the correlation equations*. This amounts to requiring that the correlation terms in (25), (26), (27) vanish. It is shown in [26] that the vanishing of correlations actually implies closure of the multi-point correlation function at all orders.

2. *The average occupations follow the discretization of the reaction diffusion equation.* Considering the reaction diffusion system (5), we approximate the laplacians with the central difference operators. We call $\rho_i^{(\alpha)}$ the density of species $\alpha \in \{0, 1, 2\}$ at vertex $i \in \{1, \dots, N\}$ with the constraint $\rho_i^{(0)} + \rho_i^{(1)} + \rho_i^{(2)} = 1$. Furthermore we fix the densities at the left end (vertex 1) to the values of $\rho_L^{(1)}, \rho_L^{(2)}$ and similarly at the right end (vertex N) we impose $\rho_R^{(1)}, \rho_R^{(2)}$. Then the discretization of the two component reaction diffusion equations (5), reads

$$\begin{aligned} \frac{d}{dt}\rho_1^{(1)} &= \sigma_{11}\left(\rho_L^{(1)} - 2\rho_1^{(1)} + \rho_2^{(1)}\right) + \sigma_{12}\left(\rho_L^{(2)} - 2\rho_1^{(2)} + \rho_2^{(2)}\right) + \Upsilon\left(\rho_1^{(2)} - \rho_1^{(1)}\right) \\ \frac{d}{dt}\rho_1^{(2)} &= \sigma_{21}\left(\rho_L^{(1)} - 2\rho_1^{(1)} + \rho_2^{(1)}\right) + \sigma_{22}\left(\rho_L^{(2)} - 2\rho_1^{(2)} + \rho_2^{(2)}\right) + \Upsilon\left(\rho_1^{(1)} - \rho_2^{(2)}\right) \end{aligned} \tag{28}$$

$$\begin{aligned} \frac{d}{dt}\rho_z^{(1)} &= \sigma_{11}\left(\rho_{z-1}^{(1)} - 2\rho_z^{(1)} + \rho_{z+1}^{(1)}\right) + \sigma_{12}\left(\rho_{z-1}^{(2)} - 2\rho_z^{(2)} + \rho_{z+1}^{(2)}\right) + \Upsilon\left(\rho_z^{(2)} - \rho_z^{(1)}\right) \\ \frac{d}{dt}\rho_z^{(2)} &= \sigma_{21}\left(\rho_{z-1}^{(1)} - 2\rho_z^{(1)} + \rho_{z+1}^{(1)}\right) + \sigma_{22}\left(\rho_{z-1}^{(2)} - 2\rho_z^{(2)} + \rho_{z+1}^{(2)}\right) + \Upsilon\left(\rho_z^{(1)} - \rho_z^{(2)}\right) \\ & \qquad \forall z = 2, \dots, N-1 \end{aligned} \tag{29}$$

$$\begin{aligned} \frac{d}{dt}\rho_N^{(1)} &= \sigma_{11}\left(\rho_{N-1}^{(1)} - 2\rho_N^{(1)} + \rho_R^{(1)}\right) + \sigma_{12}\left(\rho_{N-1}^{(2)} - 2\rho_N^{(2)} + \rho_R^{(2)}\right) + \Upsilon\left(\rho_N^{(2)} - \rho_N^{(1)}\right) \\ \frac{d}{dt}\rho_N^{(2)} &= \sigma_{21}\left(\rho_{N-1}^{(1)} - 2\rho_N^{(1)} + \rho_R^{(1)}\right) + \sigma_{22}\left(\rho_{N-1}^{(2)} - 2\rho_N^{(2)} + \rho_R^{(2)}\right) + \Upsilon\left(\rho_N^{(1)} - \rho_N^{(2)}\right) \end{aligned} \tag{30}$$

We impose that the evolution equations for the averaged occupations given in (25), (26), (27) do coincide with the discretized reaction-diffusion equations (28), (29), (30).

By imposing the closure condition 1. and the discrete linear reaction-diffusion condition 2. we get the set of equations described below.

Conditions from the bulk. We first consider Eq. (26) which we require to have the form of (29). We obtain the following conditions:

- *Closure conditions*: Equation (29) has no second order terms, thus:

$$G_{+1}^{\alpha\beta\beta'} = 0 \qquad G_{-1}^{\alpha\beta\beta'} = 0 \quad \forall \alpha, \beta, \beta' = 1, 2 \tag{31}$$

  The above requirement leads to 16 conditions on the transition rates $\Gamma_{\gamma\delta}^{\alpha\beta}$.
- *Laplacian conditions*: the one point correlation function should evolve as the coupled discrete Laplacian in (29) with linear reaction. This is accomplished by imposing:

$$\begin{aligned} &F_{-1}^{11} = F_{+1}^{11} = \sigma_{11} \quad &&F_{-1}^{12} = F_{+1}^{12} = \sigma_{12} \quad &&F_{-1}^{21} = F_{+1}^{21} = \sigma_{21} \quad &&F_{-1}^{22} = F_{+1}^{22} = \sigma_{22} \\ &F_0^{11} = -2\sigma_{11} - \Upsilon \quad &&F_0^{12} = -2\sigma_{12} + \Upsilon \quad &&F_0^{21} = -2\sigma_{21} + \Upsilon \quad &&F_0^{22} = -2\sigma_{22} - \Upsilon \end{aligned} \tag{32}$$

  The above requirement leads to 12 conditions on the transition rates $\Gamma_{\gamma\delta}^{\alpha\beta}$.
- *Zero-order terms*: Equation (29) has no zero-order term, thus:

$$E^1 = 0 \qquad E^2 = 0 \tag{33}$$

  The above requirement leads to 2 conditions on the transition rates $\Gamma_{\gamma\delta}^{\alpha\beta}$.

Our task is to determine the 81 transition rates $\Gamma^{\alpha\beta}_{\gamma\delta}$ $\forall\alpha, \beta, \gamma, \delta = 0, 1, 2$ that define the bulk infinitesimal generator. By exploiting the stochasticity properties of the generator (sum of the elements on the rows must be zero), the problem reduces to finding 72 transition rates. By considering (31), (32), (33), only $16 + 12 + 2 = 30$ conditions are available. This means that the problem to solve is under-determined.

For the analysis that will follow, it is convenient to introduce an unknown vector $\mathbf{u} \in \mathbb{R}^{72}_{+}$ that contains the desired 72 transition rates, and an appropriate matrix $K \in \mathbb{R}^{30\times 72}$ and vector $\mathbf{b} \in \mathbb{R}^{30}$. Then, it is possible (for details see Appendix C) to rewrite (31), (32), (33) as:

$$K\mathbf{u} = \mathbf{b}. \tag{34}$$

The matrix K is full rank, thus there exists a family of solutions with 42 free parameters. Furthermore we have to guarantee the non-negativity of the solution, as the transition rates are non-negative. For later use, recalling the definitions of F, G, E's, we observe that the conditions (31), (32), (33) actually only involve sums of three transition rates.

Conditions from the boundaries. We now want to find conditions to match (25) and (27) with (28) and (30), respectively. We consider the conditions on the left boundary; the right boundary is treated similarly. We get:

- *Closure conditions*: the vanishing of correlation in (25) is already guaranteed by (31).
- *Laplacian conditions*:

$$F_L^{11} + B_1^{11} = -2\sigma_{11} - \Upsilon \quad F_L^{12} + B_1^{12} = -2\sigma_{12} + \Upsilon \quad F_{+1}^{11} = \sigma_{11} \quad F_{+1}^{12} = \sigma_{12}$$
$$F_L^{22} + B_1^{22} = -2\sigma_{22} - \Upsilon \quad F_L^{21} + B_1^{21} = -2\sigma_{21} + \Upsilon \quad F_{+1}^{21} = \sigma_{21} \quad F_{+1}^{22} = \sigma_{22}$$

  Since the equations that involve $F_{+1}^{\zeta,\delta}$ are already imposed in (32), inserting the definition of the $F_L^{\zeta,\delta}$, the above conditions reduce to

$$\begin{aligned} -W_0^1(1) - W_1^0(1) - W_1^2(1) + B_1^{11} &= -2\sigma_{11} - \Upsilon \quad B_1^{12} + W_2^1(1) - W_0^1(1) \\ &= -2\sigma_{12} + \Upsilon \\ W_1^2(1) - W_0^2(1) + B_1^{21} &= -2\sigma_{21} + \Upsilon \quad - W_2^0(1) - W_0^2(1) - W_2^1(1) + B_1^{22} \\ &= -2\sigma_{22} - \Upsilon \end{aligned} \tag{35}$$

- *Zero-order terms*:

$$A_L^1 + A_1^1 = \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)} \qquad A_L^2 + A_1^2 = \sigma_{21}\rho_L^{(1)} + \sigma_{22}\rho_L^{(2)}$$

  As a consequence of (33), A_2^{ζ} are zero. Therefore, the above conditions reduce to

$$W_0^1(1) = \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)} \qquad W_0^2(1) = \sigma_{21}\rho_L^{(1)} + \sigma_{22}\rho_L^{(2)} \tag{36}$$

All in all, combining (35) and (36) we see that the rates of the boundary generators are uniquely determined by the bulk rates. Indeed, for a choice of the bulk rates (which in turn appear in the $B_1^{\zeta,\delta}$), we have:

$$\begin{aligned} &W_0^1(1) = \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)} && W_0^2(1) = \sigma_{21}\rho_L^{(1)} + \sigma_{22}\rho_L^{(2)} \\ &W_0^1(1) + W_1^0(1) + W_1^2(1) = 2\sigma_{11} + \Upsilon + B_1^{11} && W_2^1(1) - W_0^1(1) = -2\sigma_{12} + \Upsilon - B_1^{12} \\ &W_1^2(1) - W_0^2(1) = -2\sigma_{21} + \Upsilon - B_1^{21} && W_2^0(1) + W_0^2(1) + W_2^1(1) = 2\sigma_{22} + \Upsilon + B_1^{22} \end{aligned} \tag{37}$$

On the right boundary, a similar argument yields:

$$\begin{aligned}
&W_0^1(N) = \sigma_{11}\rho_R^{(1)} + \sigma_{12}\rho_R^{(2)} && W_0^2(N) = \sigma_{21}\rho_R^{(1)} + \sigma_{22}\rho_R^{(2)}\\
&W_0^1(N) + W_1^0(N) + W_1^2(N) = 2\sigma_{11} + \Upsilon + C_2^{11} && W_2^1(N) - W_0^1(N) = -2\sigma_{12} + \Upsilon - C_2^{12}\\
&W_1^2(N) - W_0^2(N) = -2\sigma_{21} + \Upsilon - C_2^{21} && W_2^0(N) + W_0^2(N) + W_2^1(N) = 2\sigma_{22} + \Upsilon + C_2^{22}
\end{aligned} \tag{38}$$

Let us notice that (37) and (38) are determined systems of algebraic equations in the unknowns $W_\cdot^\cdot(1)$, $W_\cdot^\cdot(N)$.

4.2 Determination of the Rates

Our first main result is contained in Theorem 4.1. It identifies a necessary and sufficient condition (in terms of two parameters $h, m \geq 0$) on the diffusivity matrix Σ and the reaction coefficient Υ such that the one-dimensional boundary driven chain with two-species has averaged densities satisfying the discrete linear reaction-diffusion equations (28), (29), (30). Furthermore, by setting $h = m$, it provides the example of a one-parameter family of *symmetric* models with such a property. To state the example it is convenient to introduce the *mutation map* $\alpha \mapsto \bar{\alpha}$ defined by:

$$\begin{aligned}
1 &\to 2\\
2 &\to 1\\
0 &\to 0\,.
\end{aligned} \tag{39}$$

Theorem 4.1 *Let Σ be a 2×2 positive definite diffusion matrix and $\Upsilon > 0$ be a reaction coefficient. Let $\rho_L^{(1)}$ and $\rho_L^{(2)}$ (respectively, $\rho_R^{(1)}$ and $\rho_R^{(2)}$) be the densities of the species 1 and 2 at the left (respectively, right) boundary. Then, for any choice of $h, m \geq 0$ there exist boundary-driven interacting particle systems on the chain $\{1, \dots, N\}$ such that their evolution equations of the average occupation variable are (28), (29), (30) if and only if the diffusion matrix coefficients $\sigma_{11}, \sigma_{12}, \sigma_{21}, \sigma_{22}$ and the reaction coefficient Υ are non-negative and fulfill the conditions*

$$\sigma_{11} + \sigma_{21} = \sigma_{12} + \sigma_{22} \qquad \sigma_{12} \leq \frac{\Upsilon - m}{2} \qquad \sigma_{21} \leq \frac{\Upsilon - h}{2}\,. \tag{40}$$

Moreover, an explicit example of a symmetric generator (parameterized by $h = m \geq 0$) is given by

$$L = L_1 + \sum_{x=1}^{N-1} L_{x,x+1} + L_N \tag{41}$$

with edge generator

$$\begin{aligned}
L_{x,x+1} f(\eta) = &\ \sigma_{11}(f(\eta_1, \dots, \eta_{x+1}, \eta_x, \dots, \eta_N) - f(\eta))\\
&+ \sigma_{12}(f(\eta_1, \dots, \bar{\eta}_{x+1}, \bar{\eta}_x, \dots, \eta_N) - f(\eta))\\
&+ (\Upsilon - 2\sigma_{12} - m)(f(\eta_1, \dots, \bar{\eta}_x, \eta_{x+1}, \dots, \eta_N) - f(\eta))\\
&+ m(f(\eta_1, \dots, \eta_x, \bar{\eta}_{x+1}, \dots, \eta_N) - f(\eta))\,.
\end{aligned} \tag{42}$$

The site generator at the left boundary is given by

$$
\begin{aligned}
L_1 f(\eta) = & (\sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)})\mathbb{1}_{\{\mathcal{I}_1^0\}}(\eta)\left[f(\eta_1+\delta^1,\ldots,\eta_N) - f(\eta_1,\ldots,\eta_N)\right] \\
& + (\sigma_{12}\rho_L^{(1)} + \sigma_{11}\rho_L^{(2)})\mathbb{1}_{\{\mathcal{I}_1^0\}}(\eta)\left[f(\eta_1+\delta^2,\ldots,\eta_N) - f(\eta_1,\ldots,\eta_N)\right] \\
& + (\sigma_{11}+\sigma_{12})\rho_L^{(0)}\mathbb{1}_{\{\mathcal{I}_1^1\}}(\eta)\left[f(\eta_1-\delta^1,\ldots,\eta_N) - f(\eta_1,\ldots,\eta_N)\right] \\
& + (\sigma_{11}+\sigma_{12})\rho_L^{(0)}\mathbb{1}_{\{\mathcal{I}_1^2\}}(\eta)\left[f(\eta_1-\delta^2,\ldots,\eta_N) - f(\eta_1,\ldots,\eta_N)\right] \\
& + (m + \sigma_{12}\rho_L^{(1)} + \sigma_{11}\rho_L^{(2)})\mathbb{1}_{\{\mathcal{I}_1^1\}}(\eta)\left[f(\eta_1+\delta^2-\delta^1,\ldots,\eta_N) - f(\eta_1,\ldots,\eta_N)\right] \\
& + (m + \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)})\mathbb{1}_{\{\mathcal{I}_1^2\}}(\eta)\left[f(\eta_1-\delta^2+\delta^1,\ldots,\eta_N) - f(\eta_1,\ldots,\eta_N)\right]
\end{aligned}
\tag{43}
$$

where $\rho_L^{(0)} := 1 - \rho_L^{(1)} - \rho_L^{(2)}$. Here $\pm\delta^\alpha$ denotes the addition/removal of species α. The site generator at the right boundary is defined similarly (now with parameters $\rho_R^{(1)}$ and $\rho_R^{(2)}$).

Before discussing the proof of the theorem, a few comments are collected in the following remarks.

Remark 4.2 The theorem is in agreement with the previous literature results stating that in the absence of the reaction term, for the existence of the two dimensional coupled heat equations the cross diffusivities must vanish [27, 28]. Here we find the corresponding statement at the level of the particle process. Indeed, by assuming $\Upsilon = 0$, then the condition (40) can be satisfied iff $\sigma_{12} = \sigma_{21} = h = m = 0$ and $\sigma_{11} = \sigma_{22}$.

Remark 4.3 The transitions allowed by the edge generator (42) are the following:

$$
(\gamma,\delta) \quad \rightarrow \begin{cases} (\delta,\gamma) & \text{stirring at rate } \sigma_{11} \\ (\overline{\delta},\overline{\gamma}) & \text{stirring and mutation at rate } \sigma_{12} \\ (\overline{\gamma},\delta) & \text{left mutation at rate } \Upsilon - 2\sigma_{12} - m \\ (\gamma,\overline{\delta}) & \text{right mutation at rate } m \end{cases} \tag{44}
$$

Thus we see that the rate of stirring is associated to the diffusion coefficient σ_{11}, while the rate of stirring with mutation is related to the cross-diffusion coefficient σ_{12}. The rates of the left and right mutations are precisely tuned to guarantee that, for all $m \geq 0$, the evolution equations of the average occupation variables are (28), (29), (30). A visual representation of this process is showed in Fig. 3. In particular, the choice $m = 0$ kills the right mutations, the choice $m = \Upsilon - 2\sigma_{12}$ kills the left mutations, while the choice $m = \frac{\Upsilon}{2} - \sigma_{12}$ gives the same rate to left and right mutations. Let us also observe that only when $m = 0$, the boundary generators satisfy the conditions $\forall z \in \{1, N\}$:

$$
W_1^0(z) = W_2^0(z) \qquad W_0^1(z) = W_2^1(z) \qquad W_0^2(z) = W_1^2(z)\,. \tag{45}
$$

Remark 4.4 In Theorem 4.1 we identified a one-parameter family generator. However, for fixed diffusivity matrix Σ and reaction coefficient Υ that satisfy condition (40) there exists a two-parameter ($h, m \geq 0$) family of generators with average density evolution equations given by (28),(29) and (30). In Appendix B we have written the general form of these generators, depending on the parameters $h, m \geq 0$. We observe that the rate matrix is symmetric only when $h = m$, $\sigma_{11} = \sigma_{22}$ and $\sigma_{12} = \sigma_{21}$.

Remark 4.5 Considering the "color-blind" process, i.e. the process that does not distinguish between the particles of type 1 and those of type 2, we obtain a process with just occupied or

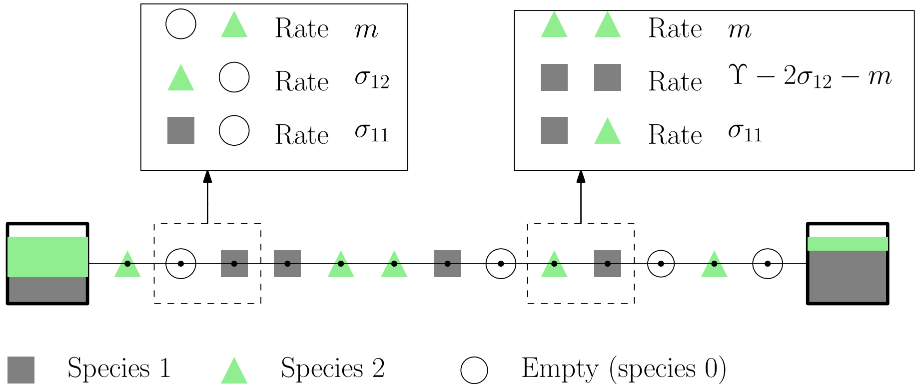

Fig. 3 The boundary driven process with generator (42), (43) . Grey squares identify species 1, green triangles species 2, and white circles the empty state. The reservoirs are represented by rectangles, where the interior colours denote the particles or vacuum densities. In the boxes, we give two examples of allowed bulk transition with the corresponding rates

empty sites. This is indeed the classical boundary-driven simple symmetric exclusion process [34], where in the bulk particles jump to the left or to the right at rate $\sigma := \sigma_{11} + \sigma_{12}$, provided there is space, and at the left boundary particles are created at rate $\sigma\rho_L$ and removed at rate $\sigma(1-\rho_L)$, where ρ_L is the particle density (and similarly at the right boundary with density ρ_R).

Proof of Theorem 4.1. We provide here the main ideas; full details of the proof are given in the appendix C. We first consider the bulk part and then the boundary one.

- *Bulk process*: To find the rates of the bulk process we need to solve (34), i.e. the system $K\mathbf{u} = \mathbf{b}$ where K is a matrix of size 30×72 and $\mathbf{b}$ is a vector described in the appendix C. This system has a great under-determination order (72-30=42). To overcome this difficulty, we exploit the fact that, as already noticed in the text following (34), the required conditions (31), (32), (33) only involve sums of three rates. As a consequence, we may introduce a new system where the unknowns are the summed triples. This new system, which will be denoted by $\Xi\mathbf{y} = \mathbf{b}$ where Ξ is a matrix of size 30×36, has an under-determination order equal to 6, and thus can be solved explicitly under the non-negativity constraint on $\mathbf{y}$ (see Appendix B). It is precisely the request $\mathbf{y} \geq 0$ that further reduces the under-determination order to 2 (parametrized by the parameters $h, m \geq 0$) and produces the constraint (40).
  Once the vector $\mathbf{y}$, whose components are sum of three rates, has been found, the next step is the identification of the transition rates themselves. This of course can be done in several ways. To produce an explicit example we have followed the two criteria below:

  – The matrix associated to the generator has the greatest number of zeros.
  – Choice of the following rates:

$$\Gamma_{12}^{21} = \sigma_{11} \qquad \Gamma_{21}^{12} = \sigma_{22} \qquad \Gamma_{11}^{22} = \sigma_{21} \qquad \Gamma_{22}^{11} = \sigma_{12}. \tag{46}$$

  After simple but long computations, this choice leads to the generator (84) in Appendix B involving the two parameters $h, m \geq 0$. When we set $h = m$ and we choose a symmetric diffusivity matrix (which in turn guarantees a symmetric particle process) the generator (42) is obtained.

- *Boundary process*: to find the rates of the boundary process we need to solve (37) and (38). Having already determined the rates of the bulk process, by direct computation we find the boundary generators (83) and (85) reported in the appendix B, which depend on $h, m \geq 0$. When we set $h = m$ and choose a symmetric diffusivity matrix, then the generator (43) is obtained.

□

5 Duality and Hydrodynamic Limit

We aim to derive the hydrodynamic equations for the family of processes defined in (42). In this section, we assume to work on the whole one-dimensional lattice $\mathbb{Z}$. To formulate the results, it is convenient to change notation. The state space of the Markov process defined by the edge generator (42) on the full line can be identified with the three-dimensional simplex

$$\widetilde{\Omega} = \left\{(n_0, n_1, n_2) \in \{0,1\}^3 \ : \ n_0 + n_1 + n_2 = 1\right\}^{\mathbb{Z}} .$$

In this notation, the component n^z at site $z \in \mathbb{Z}$ of a configuration $n \in \widetilde{\Omega}$ is thus a triplet with two 0's and a 1, whose position is associated with a hole, or with a particle of type 1, or with a particle of type 2. For example, $(n_0^z, n_1^z, n_2^z) = (0, 1, 0)$ indicates that in the site $z \in \mathbb{Z}$ there is one particle of species 1. Then, recalling the notation in (39) for the mutation map, the process $\{n(t), t \geq 0\}$ taking values in $\widetilde{\Omega}$ is defined by the following generator L working of local functions $f : \widetilde{\Omega} \to \mathbb{R}$:

$$L = \sum_{z\in\mathbb{Z}} L_{z,z+1} \tag{47}$$

with

$$L_{z,z+1} = \sigma_{11} L^{S}_{z,z+1} + \sigma_{12} L^{SM}_{z,z+1} + (\Upsilon - 2\sigma_{12} - m) L^{LM}_{z,z+1} + m L^{RM}_{z,z+1} \tag{48}$$

where

$$\begin{aligned}
L^{S}_{z,z+1} f(n) &= \sum_{\alpha,\beta=0}^{2} n_\alpha^z n_\beta^{z+1} \left[f(n - \delta_\alpha^z + \delta_\beta^z + \delta_\alpha^{z+1} - \delta_\beta^{z+1}) - f(n) \right] \\
L^{SM}_{z,z+1} f(n) &= \sum_{\alpha,\beta=0}^{2} n_\alpha^z n_\beta^{z+1} \left[f(n - \delta_\alpha^z + \delta_{\overline{\beta}}^z - \delta_\beta^{z+1} + \delta_{\overline{\alpha}}^{z+1}) - f(n) \right] \\
L^{LM}_{z,z+1} f(n) &= \sum_{\alpha=0}^{2} n_\alpha^z \left[f(n - \delta_\alpha^z + \delta_{\overline{\alpha}}^z) - f(n) \right] \\
L^{RM}_{z,z+1} f(n) &= \sum_{\beta=0}^{2} n_\beta^{z+1} \left[f(n - \delta_\beta^{z+1} + \delta_{\overline{\beta}}^{z+1}) - f(n) \right]
\end{aligned} \tag{49}$$

A fundamental tool for the hydrodynamic limit is duality: usually, the hydrodynamic limit is dictated by the scaling properties of one dual particles. We say that the Markov process with generator (47) is self-dual with respect to the self-duality function $D : \widetilde{\Omega} \times \widetilde{\Omega} \to \mathbb{R}$ if for all $t \geq 0$ and for all $(n, \ell) \in \widetilde{\Omega} \times \widetilde{\Omega}$

$$\mathbb{E}_n[D(n(t), \ell)] = \mathbb{E}_\ell[D(n, \ell(t))]$$

where on the left hand side $\mathbb{E}_n$ denotes expectation in the process $\{n(t), t \geq 0\}$ initialized from the configuration n and, analogously, on the right hand side $\mathbb{E}_\ell$ denotes expectation in $\{\ell(t), t \geq 0\}$ which is a copy of the process initialized from the configuration ℓ.

In this section, by abuse of notation, we denote $\mathbb{1}_{\{a \geq b\}}$ the function defined by

$$\mathbb{1}_{\{a\geq b\}} = \begin{cases} 1 & \text{if} \quad a \geq b \\ 0 & \text{if} \quad a < b \end{cases}$$

Theorem 5.1 (Self-Duality) *The Markov process $\{n(t), t \geq 0\}$ defined by the generator (47) is self-dual with the self duality function*

$$D(n, \ell) = \prod_{z\in\mathbb{Z}} \prod_{k=1}^{2} \mathbb{1}_{\{n_k^z \geq \ell_k^z\}} \tag{50}$$

Proof It is enough to prove that

$$(LD(\cdot, \ell))\,(n) = (LD(n, \cdot))\,(\ell) \qquad \forall (n, \ell) \in \widetilde{\Omega} \times \widetilde{\Omega} \tag{51}$$

The generator (47) is a superposition of four generators. Remarkably, the duality relation can be verified for each of them. Indeed, one has:

$$\begin{aligned}
&(L^S_{z,z+1} D(\cdot, \ell))(n) \\
&= \Big[\mathbb{1}_{\{n_1^{z+1} \geq \ell_1^z\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_2^z\}} \mathbb{1}_{\{n_1^z \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_2^z \geq \ell_2^{z+1}\}} \\
&- \mathbb{1}_{\{n_1^z \geq \ell_1^z\}} \mathbb{1}_{\{n_2^z \geq \ell_2^z\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_2^{z+1}\}}\Big] \prod_{x \notin \{z,z+1\}} \prod_{k=1}^{2} \mathbb{1}_{\{n_k^x \geq \ell_k^x\}} \\
&= \Big[\mathbb{1}_{\{n_1^z \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_2^z \geq \ell_2^{z+1}\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_1^z\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_2^z\}} \\
&- \mathbb{1}_{\{n_1^z \geq \ell_1^z\}} \mathbb{1}_{\{n_2^z \geq \ell_2^z\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_2^{z+1}\}}\Big] \prod_{x \notin \{z,z+1\}} \prod_{k=1}^{2} \mathbb{1}_{\{n_k^x \geq \ell_k^x\}} \\
&= (L^S_{z,z+1} D(n, \cdot))(\ell)\,.
\end{aligned}$$

Similarly, one has

$$\begin{aligned}
&(L^{SM}_{z,z+1} D(\cdot, \ell))(n) \\
&= \Big[\mathbb{1}_{\{n_2^{z+1} \geq \ell_1^z\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_2^z\}} \mathbb{1}_{\{n_2^z \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_1^z \geq \ell_2^{z+1}\}} \\
&- \mathbb{1}_{\{n_1^z \geq \ell_1^z\}} \mathbb{1}_{\{n_2^z \geq \ell_2^z\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_2^{z+1}\}}\Big] \prod_{x \notin \{z,z+1\}} \prod_{k=1}^{2} \mathbb{1}_{\{n_k^x \geq \ell_k^x\}} \\
&= \Big[\mathbb{1}_{\{n_1^z \geq \ell_2^{z+1}\}} \mathbb{1}_{\{n_2^z \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_2^z\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_1^z\}} \\
&- \mathbb{1}_{\{n_1^z \geq \ell_1^z\}} \mathbb{1}_{\{n_2^z \geq \ell_2^z\}} \mathbb{1}_{\{n_1^{z+1} \geq \ell_1^{z+1}\}} \mathbb{1}_{\{n_2^{z+1} \geq \ell_2^{z+1}\}}\Big] \prod_{x \notin \{z,z+1\}} \prod_{k=1}^{2} \mathbb{1}_{\{n_k^x \geq \ell_k^x\}} \\
&= L^{SM}_{z,z+1} (D(n, \cdot)(\ell)\,.
\end{aligned}$$

For the generator that mutates at site z we have

$$\begin{aligned}(L^{LM}_{z,z+1}D(\cdot,\ell))(n) &= \left[\mathbb{1}_{\{n^z_2\ge\ell^z_1\}}\mathbb{1}_{\{n^z_1\ge\ell^z_2\}} - \mathbb{1}_{\{n^z_1\ge\ell^z_1\}}\mathbb{1}_{\{n^z_2\ge\ell^z_2\}}\right]\prod_{x\neq z}\prod_{k=1}^{2}\mathbb{1}_{\{n^x_k\ge\ell^x_k\}}\\ &= \left[\mathbb{1}_{\{n^z_1\ge\ell^z_2\}}\mathbb{1}_{\{n^z_2\ge\ell^z_1\}} - \mathbb{1}_{\{n^z_1\ge\ell^z_1\}}\mathbb{1}_{\{n^z_2\ge\ell^z_2\}}\right]\prod_{x\neq z}\prod_{k=1}^{2}\mathbb{1}_{\{n^x_k\ge\ell^x_k\}}\\ &= (L^{LM}_{z,z+1}D(n,\cdot))(\ell)\,,\end{aligned}$$

and analogously, for the generator that mutates at site $z+1$, we find

$$\begin{aligned}(L^{RM}_{z,z+1}D(\cdot,\ell))(n) &= \left[\mathbb{1}_{\{n^{z+1}_2\ge\ell^{z+1}_1\}}\mathbb{1}_{\{n^{z+1}_1\ge\ell^{z+1}_2\}} - \mathbb{1}_{\{n^{z+1}_1\ge\ell^{z+1}_1\}}\mathbb{1}_{\{n^{z+1}_2\ge\ell^{z+1}_2\}}\right]\prod_{x\neq z+1}\prod_{k=1}^{2}\mathbb{1}_{\{n^x_k\ge\ell^x_k\}}\\ &= \left[\mathbb{1}_{\{n^{z+1}_1\ge\ell^{z+1}_2\}}\mathbb{1}_{\{n^{z+1}_2\ge\ell^{z+1}_1\}} - \mathbb{1}_{\{n^{z+1}_1\ge\ell^{z+1}_1\}}\mathbb{1}_{\{n^{z+1}_2\ge\ell^{z+1}_2\}}\right]\prod_{x\neq z+1}\prod_{k=1}^{2}\mathbb{1}_{\{n^x_k\ge\ell^x_k\}}\\ &= (L^{RM}_{z,z+1}D(n,\cdot)(\ell)\end{aligned}$$

□

Remark 5.2 It is interesting to notice that to ensure the existence of a dual process, closure condition (31) is not enough. Considering the most general reaction-diffusion process satisfying closed equations, described by the generator $\mathcal{L}_{z,z+1}$ in (84), we have to further assume that

$$\sigma_{22} = \sigma_{11} \qquad \sigma_{21} = \sigma_{12} \qquad h = m. \tag{52}$$

Indeed, the duality relation (51) is equivalent to the following relation between matrices

$$(d\otimes d)^{-1}\,\mathcal{L}_{z,z+1}\,(d\otimes d) = \widetilde{L}^T_{z,z+1} \qquad \forall z\in\mathbb{Z} \tag{53}$$

where ^{T} denotes transposition and where

$$d = \begin{pmatrix}1&0&0\\1&1&0\\1&0&1\end{pmatrix} \tag{54}$$

In order to interpret $\widetilde{L}_{z,z++1}$ as a generator of a stochastic particle system, we have to impose that the out of diagonal elements are non-negative and the sum of the elements of each row is equal to zero. It is possible to show that this is equivalent to requiring that (52) holds. Moreover, if (52) is fulfilled, both the matrices $\mathcal{L}_{z,z+1}$ and $\widetilde{L}_{z,z+1}$ do coincide with the matrix associated to the generator $L_{z,z+1}$ given in (48), i.e. self-duality.

To formulate the hydrodynamic limit, we consider a scaling parameter $\epsilon \geq 0$ and we introduce the empirical density fields

$$X^\epsilon_1(t) = \epsilon\sum_{z\in\mathbb{Z}} n^z_1(\epsilon^{-2}t)\delta_{\epsilon z} \qquad X^\epsilon_2(t) = \epsilon\sum_{z\in\mathbb{Z}} n^z_2(\epsilon^{-2}t)\delta_{\epsilon z} \tag{55}$$

The empirical density fields $\{X^\epsilon_1(t), t\geq 0\}$ and $\{X^\epsilon_2(t), t\geq 0\}$ are measure-valued processes constructed from the process $\{n(t), t\geq 0\}$. We also need to specify a good set of initial distributions.

Definition 5.3 Let $\widehat{\rho}^{(\alpha)} : \mathbb{R} \to [0,1]$, with $\alpha \in \{1,2\}$, be a continuous bounded real function called the initial macroscopic profile. A sequence $(\mu_\epsilon)_{\epsilon \geq 0}$ of measures on $\widetilde{\Omega}$, is a sequence of compatible initial conditions if $\forall \alpha \in \{1,2\}$, $\forall \delta > 0$:

$$\lim_{\epsilon \to 0} \mu_\epsilon \left(\left| \langle X_\alpha^\epsilon(0), g \rangle - \int_{\mathbb{R}} g(x) \widehat{\rho}^{(\alpha)}(x) dx \right| > \delta \right) = 0 \tag{56}$$

where $g : \mathbb{R} \to \mathbb{R}$ is a smooth test function with compact support.

We then have the following theorem for the hydrodynamic limit.

Theorem 5.4 (Hydrodynamic limit of the Markov process $\{n(t), t \geq 0\}$). *Let $\widehat{\rho}^{(\alpha)}$ with $\alpha \in \{1,2\}$ be initial macroscopic profiles and $(\mu_\epsilon)_{\epsilon>0}$ be a sequence of compatible initial conditions. Let $\mathbb{P}_{\mu_\epsilon}$ be the law of the measure valued process $(X_1^\epsilon(t), X_2^\epsilon(t))$ defined in (55). Then $\forall T, \delta > 0, \forall \alpha \in \{1,2\}$ and for all smooth test function with compact support $g : \mathbb{R} \to \mathbb{R}$*

$$\lim_{\epsilon \to 0} \mathbb{P}_{\mu_\epsilon} \left(\sup_{t \in [0,T]} \left| \langle X_\alpha^\epsilon(t), g \rangle - \int_{\mathbb{R}} g(x) \rho^{(\alpha)}(x,t) dx \right| > \delta \right) = 0, \tag{57}$$

where $\rho^{(1)}$, $\rho^{(2)}$ are the strong solutions of

$$\begin{cases} \partial_t \rho^{(1)} = \sigma_{11} \partial_x^2 \rho^{(1)} + \widetilde{\Upsilon} \left(\rho^{(2)} - \rho^{(1)} \right) \\ \partial_t \rho^{(2)} = \sigma_{11} \partial_x^2 \rho^{(2)} + \widetilde{\Upsilon} \left(\rho^{(1)} - \rho^{(2)} \right) \\ \rho^{(\alpha)}(0,x) = \widehat{\rho}^{(\alpha)}(x) \qquad \forall x \in [0,1], \ \forall \alpha \in \{1,2\} \end{cases} \tag{58}$$

Proof The proof is standard and it is based on the Dynkin's martingale and its quadratic variation. For the tightness and the uniqueness of the limiting point we refer to [23] and [35]. we provide here some details for the computations of the Dynkin's martingale and its quadratic variation via Carré-Du-Champ.

We introduce the following real and positive parameters:

$$\widetilde{\sigma}_{12} = \epsilon^{-2} \sigma_{12}, \quad \widetilde{\Upsilon} = \epsilon^{-2} \Upsilon \quad \widetilde{m} = \epsilon^{-2} m. \tag{59}$$

We consider the re-scaled generator

$$L^{(\epsilon)} = \sum_{z \in \mathbb{Z}} L_{z,z+1}^{(\epsilon)} \tag{60}$$

where

$$L_{z,z+1}^{(\epsilon)} = \sigma_{11} L_{z,z+1}^{S} + \widetilde{\sigma}_{12} \epsilon^2 L_{z,z+1}^{SM} + \epsilon^2 (\widetilde{\Upsilon} - 2\widetilde{\sigma}_{12} - \widetilde{m}) L_{z,z+1}^{LM} + \widetilde{m} \epsilon^2 L_{z,z+1}^{RM}. \tag{61}$$

By choosing $\forall z \in \mathbb{Z}$ and $\forall \alpha \in \{1,2\}$ the action of the rescaled generator on n_α^z is the following:

$$\begin{aligned} (L^{(\epsilon)} n_\alpha^x)(n) &= \sigma_{11} \left(n_\alpha^{z+1} - 2n_\alpha^z + n_\alpha^{z-1} \right) \\ &\quad + \widetilde{\sigma}_{12} \epsilon^2 \left(n_{\overline{\alpha}}^{z+1} - 2n_\alpha^z + n_{\overline{\alpha}}^{z-1} \right) + \epsilon^2 \left(\widetilde{\Upsilon} - 2\widetilde{\sigma}_{12} \right) \left(n_{\overline{\alpha}}^z - n_\alpha^z \right) \end{aligned}$$

By consequence considering a test function g

$$\begin{aligned} &\int_0^t ds \, \epsilon^{-2} L^{(\epsilon)} \langle X_\alpha^\epsilon(s), g \rangle \\ &= \sigma_{11} \int_0^t ds \, \epsilon^{-2} \, \epsilon \sum_{z \in \mathbb{Z}} n_\alpha^z(s) \left[g\left((z+1)\epsilon\right) - 2g\left(z\epsilon\right) + g\left((z-1)\epsilon\right) \right] \end{aligned}$$

$$+\widetilde{\sigma}_{12}\int_0^t ds\ \epsilon^{-2}\epsilon^3 \sum_{z\in\mathbb{Z}}\left(n^z_{\overline{\alpha}}(s)\left[g\left((z+1)\epsilon\right)+g\left((z-1)\epsilon\right)\right]-2n^z_\alpha(s)g(z\epsilon)\right)$$
$$+\int_0^t ds\ \epsilon^{-2}\ \epsilon^3(\widetilde{\Upsilon}-2\widetilde{\sigma}_{12})\sum_{z\in\mathbb{Z}} g\left(z\epsilon\right)\left[n^z_{\overline{\alpha}}-n^z_\alpha\right]$$

By using the Taylor expansion we rewrite the above equality as

$$\begin{aligned}\int_0^t ds\ \epsilon^{-2}L^{(\epsilon)}\langle X^\epsilon_\alpha(s),g\rangle &= \sigma_{11}\int_0^t \epsilon\sum_{z\in\mathbb{Z}} n^z_\alpha\Delta g\left(z\epsilon\right)\\ &\quad+\widetilde{\sigma}_{12}\int_0^t \epsilon^3\sum_{z\in\mathbb{Z}} n^z_{\overline{\alpha}}\Delta g\left(z\epsilon\right)+\widetilde{\Upsilon}\int_0^t \epsilon\sum_{z\in\mathbb{Z}} g\left(z\epsilon\right)\left[n^z_{\overline{\alpha}}-n^z_\alpha\right]\\ &\quad+o(\epsilon)\\ &=\sigma_{11}\int_0^t \epsilon\sum_{z\in\mathbb{Z}} n^z_\alpha\Delta g\left(z\epsilon\right)+\widetilde{\Upsilon}\int_0^t \epsilon\sum_{z\in\mathbb{Z}} g\left(z\epsilon\right)\left[n^z_{\overline{\alpha}}-n^z_\alpha\right]+o(\epsilon).\end{aligned}$$

Defining the Dynkin's martingale $\forall\alpha\in\{1,2\}$

$$M^t_g(X^\epsilon_\alpha):=\langle X^\epsilon_\alpha(t),g\rangle-\langle X^\epsilon_\alpha(0),g\rangle-\int_0^t \epsilon^{-2}L^{(\epsilon)}\langle X^\epsilon_\alpha(s),g\rangle ds, \tag{62}$$

by the previous computations, we have

$$\begin{aligned}M^t_g(X^\epsilon_\alpha)+o(\epsilon)&=\langle X^\epsilon_\alpha(t),g\rangle-\langle X^\epsilon_\alpha(0),g\rangle\\ &\quad-\sigma_{11}\int_0^t\langle X^\epsilon_\alpha(s),\Delta g\rangle ds-\widetilde{\Upsilon}\int_0^t\langle X^\epsilon_{\overline{\alpha}}(s)-X^\epsilon_\alpha(s),g\rangle ds.\end{aligned}$$

The right-hand side is the discrete counterpart of the weak solution of (58).

To have tightness of the law of the measure-valued processes (55) we need to show that

$$\lim_{\epsilon\to 0}\mathbb{E}_{\mu_\epsilon}\left[M^t_g(X^\epsilon_\alpha)^2\right]=0. \tag{63}$$

We first observe that

$$\begin{aligned}\mathbb{E}_{\mu_\epsilon}\left[M^t_g(X^\epsilon_\alpha)^2\right]&\le\mathbb{E}_{\mu_\epsilon}\left[\sup_{t\in[0,T]}|M^t_g(X^\epsilon_\alpha)|^2\right]\\ &\le 4\mathbb{E}_{\mu_\epsilon}\left[M^T_g(X^\epsilon_\alpha)^2\right]=4\mathbb{E}_{\mu_\epsilon}\left[\int_0^T\epsilon^{-2}\Gamma^s_g(X^\epsilon_\alpha)ds\right],\end{aligned}$$

where $\Gamma^s_g(X^\epsilon_\alpha)$ is the Carré-Du-Champ operator that can be written as

$$\Gamma^s_g(X^\epsilon_\alpha)=L^{(\epsilon)}\langle X_\alpha(t),g\rangle^2-2\langle X_\alpha(t),g\rangle L^{(\epsilon)}\langle X_\alpha(t),g\rangle. \tag{64}$$

By using the definition of the re-scaled generator (61) we obtain the following

$$\begin{aligned}\epsilon^{-2}\Gamma_g^s(X_\alpha^\epsilon) &= \sigma_{11}\epsilon^2\sum_{z\in\mathbb{Z}}\left[n_\alpha^z(1-n_\alpha^{z+1})+n_{\bar\alpha}^z(1-n_{\bar\alpha}^{z+1})\right](\nabla g(z\epsilon))^2\\ &+\widetilde{\sigma}_{12}\epsilon^2\sum_{z\in\mathbb{Z}}\Big\{2\left[n_\alpha^z n_{\bar\alpha}^{z+1}+n_{\bar\alpha}^z n_\alpha^{z+1}\right]g(z\epsilon)g((z+1)\epsilon)\\ &+n_{\bar\alpha}^z\left[g((z+1)\epsilon)^2+g((z-1)\epsilon)^2\right]+n_\alpha^z 2g(z\epsilon)^2\Big\}\\ &+\left(\widetilde{\Upsilon}-2\widetilde{\sigma}_{12}\right)\epsilon^2\sum_{z\in\mathbb{Z}}(n_{\bar\alpha}^z+n_\alpha^z)g(z\epsilon)^2+o(\epsilon^2).\end{aligned} \tag{65}$$

Let's introduce the set $\mathcal{S}_g$ as the smallest compact subset of $\mathbb{R}$ that contains the supports of a fixed g and of the first two derivatives. Then, $|\mathcal{S}_g|\leq C'\epsilon^{-1}$, with a C' positive and finite constant. Moreover, by the hard-core constraint $n_\alpha^z\leq 1$, $\forall z\in\mathbb{Z}$ and $\forall\alpha\in\{1,2\}$. By consequence, exploiting the smoothness of g we derive the following bound

$$\mathbb{E}_{\mu_\epsilon}\left[\int_0^T\epsilon^{-2}\Gamma_g^s(X_\alpha^\epsilon)ds\right]\leq C\epsilon, \tag{66}$$

with $C<\infty$. This concludes the proof. □

Remark 5.5 Let's define a "color-blind" density field

$$X^\epsilon(t):=\epsilon\sum_{z\in\mathbb{Z}}n^z(t\epsilon^{-2})\delta_{z\epsilon} \tag{67}$$

where $n^z(t):=n_\alpha^z(t)+n_{\bar\alpha}^z(t)$. By re-scaling only the $L_{z,z+1}^{RM}$ and $L_{z,z+1}^{LM}$ terms of the generator, the same proof of Theorem 5.4 we would give, as limiting PDE, the heat equation

$$\begin{cases}\partial_t\rho(x,t)=(\sigma_{11}+\sigma_{12})\partial_{xx}\rho(x,t)\\ \rho(x,0)=\rho_0(x)\end{cases} \tag{68}$$

This is in agreement with the Remark 4.5.

Remark 5.6 We observe that in order to obtain the hydrodynamic limit of the process $\{n(t);t\geq 0\}$ we had to scale the parameters as in (59). Indeed, the 'naive' scaling where the diffusivity parameters σ_{11} and σ_{12} are both kept constant (while the reaction parameters are scaled as $\Upsilon=\epsilon^2\tilde{\Upsilon}$ and $m=\epsilon^2\tilde{m}$) is not viable as it would make (65) infinite when $\epsilon\to 0$. In other words, the problem with the 'naive' rescaling is that the rate of left mutations

$$(\widetilde{\Upsilon}\epsilon^2-2\sigma_{12}-\widetilde{m}\epsilon^2) \tag{69}$$

becomes negative (!) for sufficiently small ϵ. One could still wonder if other scalings of the parameters would lead to Eq. (5) in the hydrodynamic limit. We argue that this is not possible, because the maximum principle (which is a necessary condition for the Markov property) would be violated. To show this, we rewrite the PDEs (5) in the form

$$\begin{cases}\partial_t\begin{pmatrix}\rho^{(1)}\\ \rho^{(2)}\end{pmatrix}=A\begin{pmatrix}\rho^{(1)}\\ \rho^{(2)}\end{pmatrix} \qquad \forall x\in[0,1]\\ \rho^{(1)}(0,x)=\widehat{\rho}^{(1)}(x),\quad \rho^{(2)}(0,x)=\widehat{\rho}^{(2)}(x)\end{cases} \tag{70}$$

where the operator A is defined as

$$A:=\begin{pmatrix}\sigma_{11}\partial_{xx} & \sigma_{12}\partial_{xx}\\ \sigma_{12}\partial_{xx} & \sigma_{11}\partial_{xx}\end{pmatrix}+\Upsilon\begin{pmatrix}-1 & 1\\ 1 & -1\end{pmatrix} \tag{71}$$

Now, for a function $f = (f^{(1)}, f^{(2)})$ in the domain of A, let $x_* \in (0, 1)$ be such that

$$f^{(1)}(x_*) := \max_{x\in(0,1)} f^{(1)}(x) \tag{72}$$

Then the first component of $(Af)(x_*)$ reads

$$\sigma_{11}\partial_{xx} f^{(1)}(x_*) + \sigma_{12}\partial_{xx} f^{(2)}(x_*) + \widetilde{\Upsilon}\left(f^{(2)}(x_*) - f^{(1)}(x_*)\right). \tag{73}$$

Clearly (73) can be positive, since (72) guarantees that $\partial_{xx} f^{(1)}(x^*) \le 0$, but the other terms of (73) can be positive and arbitrary large. As a consequence of the violation of the maximum principle it follows that A can not be the generator of a Markov process.

Remark 5.7 If we perform the hydrodynamic limit with an "Euler" re-scaling, i.e. we re-scale the time only by a factor ϵ and we define $\widehat{\sigma}_{12} = \epsilon^{-1}\sigma_{12}$, $\widehat{\Upsilon} = \epsilon^{-1}\Upsilon$ and $\widetilde{m} = \epsilon^{-1}m$ we obtain the following ODE's system

$$\begin{cases} \frac{d}{dt}\rho^{(1)}(t) = \widehat{\Upsilon}(\rho^{(2)} - \rho^{(1)}) \\ \frac{d}{dt}\rho^{(2)}(t) = \widehat{\Upsilon}(\rho^{(1)} - \rho^{(2)}) \\ \rho^{(1)}(0) = \rho_0^{(1)}, \quad \rho^{(2)}(0) = \rho_0^{(2)} \end{cases} \tag{74}$$

that is a purely reacting system. The ODE's are linear and the solution is given by

$$\begin{cases} \rho^{(1)}(t) = \frac{\rho_0^{(1)}+\rho_0^{(2)}}{2} + \frac{\rho_0^{(1)}-\rho_0^{(2)}}{2}e^{-2\widehat{\Upsilon}t} \\ \rho^{(2)}(t) = \frac{\rho_0^{(1)}+\rho_0^{(2)}}{2} - \frac{\rho_0^{(1)}-\rho_0^{(2)}}{2}e^{-2\widehat{\Upsilon}t} \end{cases} \tag{75}$$

6 Conclusions

We considered multi-species stochastic interacting particle systems with hard-core interaction defined on a directed graph. We also added site-generators, that allow to define the boundary-driven version having non-zero stationary currents.

For a one dimensional chain with two species, we established that in order to have that the average occupation evolves as the discrete counterpart of the linear reaction-diffusion equation (5), the diffusivity matrix Σ and the reaction coefficient Υ have to fulfill condition (40) of Theorem 4.1. As an additional result, we have identified a one-parameter family of multi-species interacting particle systems (the one defined by the generator (42)) where the analysis can be pushed further. In particular, due to the existence of a dual process, the hydrodynamic limit is deduced. In the hydrodynamic regime the coupling between species due to the cross-diffusivity coefficients disappears. The origin of this is that if the cross-diffusivities are not scaled to zero then the Markov property is lost (see Remark 5.6). Partial uphill diffusion, although present in a finite size system, is lost in the hydrodynamic limit.

It would be interesting to extend the analysis to a higher number of species. As observed in [9–11] the uphill phenomenology of systems with three species of particles or more can be substantially different from the ones with two species. Another open problem is the study of uphill diffusion for systems with a *non-linear* reaction-diffusion system, i.e. with diffusivity matrix whose elements are functions of the particle densities [29]. Finally, we mention that the family of models with generator (42) includes the stirring process which is known to possess the algebraic structure of the $GL(n)$ group (which in fact leads to integrability of the model [36]). It would be interesting to check if the model we have introduced preserves such algebraic structure.

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Declarations

Conflict of interest The authors have no conflicts of interest.

A Steady State Partial Uphill Diffusion

Non Diagonal Diffusivity Matrix Equation

We shall show that in this set up partial uphill diffusion is possible. To this aim, because of the great number of parameters we specialize (10) to a particular choice, namely

$$\sigma_{11} = \sigma_{22} = \Upsilon = 1 \qquad \sigma_{21} = \sigma_{12} = \frac{1}{2}\,. \tag{76}$$

The stationary profiles become

$$\begin{aligned}\rho^{(\zeta)}(x) =& \frac{\rho_L^{(1)}}{2} + \frac{\rho_L^{(2)}}{2} - \frac{x\left(\rho_L^{(1)} + \rho_L^{(2)} - \rho_R^{(1)} - \rho_R^{(2)}\right)}{2} \\ &+ (-1)^\zeta \frac{\mathrm{e}^{2-2x}\left(\rho_R^{(1)} - \rho_R^{(2)} - \rho_L^{(1)}\,\mathrm{e}^2 + \rho_L^{(2)}\,\mathrm{e}^2\right)}{2\left(\mathrm{e}^4 - 1\right)} \\ &+ (-1)^\zeta \frac{\mathrm{e}^{2x}\left(\rho_L^{(1)} - \rho_L^{(2)} - \rho_R^{(1)}\,\mathrm{e}^2 + \rho_R^{(2)}\,\mathrm{e}^2\right)}{2\left(\mathrm{e}^4 - 1\right)} \qquad \forall \zeta = 1, 2\end{aligned} \tag{77}$$

and the diffusive currents read

$$
\begin{aligned}
J^{(\zeta)}(x) =& \frac{3\,\rho_L^{(1)}}{4} + \frac{3\,\rho_L^{(2)}}{4} - \frac{3\,\rho_R^{(1)}}{4} - \frac{3\,\rho_R^{(2)}}{4} \\
&+ (-1)^{\zeta} \frac{\mathrm{e}^{2-2x}\left(\rho_R^{(1)} - \rho_R^{(2)} - \rho_L^{(1)}\,\mathrm{e}^2 + \rho_L^{(2)}\,\mathrm{e}^2\right)}{2\left(\mathrm{e}^4 - 1\right)} \\
&- (-1)^{\zeta} \frac{\mathrm{e}^{2x}\left(\rho_L^{(1)} - \rho_L^{(2)} - \rho_R^{(1)}\,\mathrm{e}^2 + \rho_R^{(2)}\,\mathrm{e}^2\right)}{2\left(\mathrm{e}^4 - 1\right)} \qquad \forall \zeta = 1, 2
\end{aligned} \tag{78}
$$

The problem of having partial uphill for, say, the species 1 is then the following: by assuming that $\rho_L^{(1)} < \rho_R^{(1)}$

$$
\text{find} \quad (\rho_L^{(1)}, \rho_L^{(2)}, \rho_R^{(1)}, \rho_R^{(2)}) \quad \text{such that} \quad \min_{x \in [0,1]} J^{(1)}(x) > 0. \tag{79}
$$

There are choices of boundary densities that allow for partial uphill diffusion of the species 1. We give an example in Fig. 1.

Diagonal Diffusivity Matrix Equations

We specialize the stationary solution (10) to the case where $\sigma_{12} = \sigma_{21} = 0$ and $\Upsilon > 0$. Motivated by the hydrodynamic result (58), we consider the case $\sigma_{11} = \sigma_{22}$. Introducing the constant $k^2 = \frac{\Upsilon}{\sigma_{11}}$, the stationary profiles takes the form:

$$
\begin{aligned}
\rho^{(\zeta)}(x) = \frac{1}{2} \Big(& \rho_L^{(1)} + \rho_L^{(2)} + x(-\rho_L^{(1)} - \rho_L^{(2)} + \rho_R^{(1)} + \rho_R^{(2)}) \\
& - (-1)^{\zeta} \operatorname{csch}\left(\sqrt{2}k\right) \Big((\rho_L^{(2)} - \rho_L^{(1)}) \sinh\left(\sqrt{2}k(x-1)\right) \\
& + (\rho_R^{(1)} - \rho_R^{(2)}) \sinh\left(\sqrt{2}kx\right)\Big)\Big) \qquad \forall \zeta = 1, 2
\end{aligned} \tag{80}
$$

The diffusive currents then read:

$$
\begin{aligned}
J^{(\zeta)}(x) =& \frac{1}{2} \Big(\rho_L^{(1)} + \rho_L^{(2)} - \rho_R^{(1)} - \rho_R^{(2)} + \\
& + (-1)^{\zeta} \sqrt{2}k \operatorname{csch}\left(\sqrt{2}k\right) \Big((\rho_L^{(2)} - \rho_L^{(1)}) \cosh\left(\sqrt{2}k(x-1)\right) \\
& + (\rho_R^{(1)} - \rho_R^{(2)}) \cosh\left(\sqrt{2}kx\right)\Big)\Big) \qquad \forall \zeta = 1, 2
\end{aligned} \tag{81}
$$

The problem of having partial uphill for, say, the species 1 is then the following: by assuming that $\rho_L^{(1)} < \rho_R^{(1)}$

$$
\text{find} \quad (\rho_L^{(1)}, \rho_L^{(2)}, \rho_R^{(1)}, \rho_R^{(2)}) \quad \text{such that} \quad \min_{x \in [0,1]} J^{(1)}(x) > 0. \tag{82}
$$

One can check that $\forall k > 0$ and $\forall \rho_L^{(1)}, \rho_L^{(2)}, \rho_R^{(1)}, \rho_R^{(2)}$ such that $\rho_L^{(1)} < \rho_R^{(1)}$, the minimum of $J^{(1)}(x)$ is always negative. By consequence, partial uphill cannot occur for (58).

A similar analysis can be done for the discretized equations (28), (29), (30).

B A Two-Parameter Family of Models

In the following we report the matrices that describe the two-parameter family of generators introduced in Remark 4.4. The matrices representing the generators $\mathcal{L}_{z,z+1}$ are of dimension 9×9 while the matrices representing the generators $\mathcal{L}_1,\ \mathcal{L}_N$ are of dimension 3×3. The elements of these matrices are ordered as follows:

- for $\mathcal{L}_{z,z+1}$, the row and the column indexes are

$$00, 01, 02, 10, 11, 12, 20, 21, 22$$

  For example, the element on the 3rd row and 4th column gives the rate of transition $02 \to 10$
- for the site matrices $\mathcal{L}_1$ and $\mathcal{L}_N$, the rows and the columns a indexes are 0, 1, 2.

$$\mathcal{L}_1 = \begin{pmatrix} -\sigma_{11}\rho_L^{(1)} - \sigma_{12}\rho_L^{(2)} - \sigma_{21}\rho_L^{(1)} - \sigma_{22}\rho_L^{(2)} & \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)} & \sigma_{21}\rho_L^{(1)} + \sigma_{22}\rho_L^{(2)} \\ \sigma_{11} + \sigma_{21} - \sigma_{11}\rho_L^{(1)} - \sigma_{12}\rho_L^{(2)} - \sigma_{21}\rho_L^{(1)} - \sigma_{22}\rho_L^{(2)} & \sigma_{11}\rho_L^{(1)} - \sigma_{21} - h - \sigma_{11} + \sigma_{12}\rho_L^{(2)} & h + \sigma_{21}\rho_L^{(1)} + \sigma_{22}\rho_L^{(2)} \\ \sigma_{22} + \sigma_{12} - \sigma_{22}\rho_L^{(2)} - \sigma_{21}\rho_L^{(1)} - \sigma_{12}\rho_L^{(2)} - \sigma_{11}\rho_L^{(1)} & m + \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)} & \sigma_{21}\rho_L^{(1)} - \sigma_{12} - m - \sigma_{22} + \sigma_{22}\rho_L^{(2)} \end{pmatrix} \tag{83}$$

$$\mathcal{L}_{z,z+1} = \begin{pmatrix} \Gamma_{00}^{00} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \Gamma_{01}^{01} & h & \sigma_{11} & 0 & 0 & \sigma_{21} & 0 & 0 \\ 0 & m & \Gamma_{02}^{02} & \sigma_{12} & 0 & 0 & \sigma_{22} & 0 & 0 \\ 0 & \sigma_{11} & \sigma_{21} & \Gamma_{10}^{10} & 0 & 0 & \Upsilon - 2\sigma_{21} - h & 0 & 0 \\ 0 & 0 & 0 & 0 & \Gamma_{11}^{11} & h & 0 & \Upsilon - 2\sigma_{21} - h & \sigma_{21} \\ 0 & 0 & 0 & 0 & m & \Gamma_{12}^{12} & 0 & \sigma_{11} & \Upsilon - \sigma_{12} - \sigma_{21} - h \\ 0 & \sigma_{12} & \sigma_{22} & \Upsilon - 2\sigma_{12} - m & 0 & 0 & \Gamma_{20}^{20} & 0 & 0 \\ 0 & 0 & 0 & 0 & \Upsilon - \sigma_{12} - \sigma_{21} - m & \sigma_{22} & 0 & \Gamma_{21}^{21} & h \\ 0 & 0 & 0 & 0 & \sigma_{12} & \Upsilon - 2\sigma_{12} - m & 0 & m & \Gamma_{22}^{22} \end{pmatrix} \tag{84}$$

Due to the stochasticity of the generator, the diagonal elements are the following

$$\begin{aligned} &\Gamma_{00}^{00} = 0 && \Gamma_{01}^{01} = -\sigma_{11} - \sigma_{21} - h && \Gamma_{02}^{02} = -\sigma_{22} - \sigma_{12} - m \\ &\Gamma_{10}^{10} = -\Upsilon - \sigma_{11} + \sigma_{21} + h && \Gamma_{11}^{11} = -\Upsilon + \sigma_{21} && \Gamma_{12}^{12} = -\sigma_{11} - \Upsilon + \sigma_{12} + \sigma_{21} - m + h \\ &\Gamma_{20}^{20} = -\Upsilon - \sigma_{22} + \sigma_{12} + m && \Gamma_{21}^{21} = -\Upsilon - \sigma_{22} + \sigma_{21} + \sigma_{12} + m - h && \Gamma_{22}^{22} = -\Upsilon + \sigma_{12} \end{aligned}$$

$$\mathcal{L}_N = \begin{pmatrix} -\sigma_{11}\rho_R^{(1)} - \sigma_{12}\rho_R^{(2)} - \sigma_{21}\rho_R^{(1)} - \sigma_{22}\rho_R^{(2)} & \sigma_{11}\rho_R^{(1)} + \sigma_{12}\rho_R^{(2)} & \sigma_{21}\rho_R^{(1)} + \sigma_{22}\rho_R^{(2)} \\ \sigma_{11} + \sigma_{21} - \sigma_{11}\rho_R^{(1)} - \sigma_{12}\rho_R^{(2)} - \sigma_{21}\rho_R^{(1)} - \sigma_{22}\rho_R^{(2)} & \sigma_{11}\rho_R^{(1)} - \sigma_{21} - h - \sigma_{11} + \sigma_{12}\rho_R^{(2)} & h + \sigma_{21}\rho_R^{(1)} + \sigma_{22}\rho_R^{(2)} \\ \sigma_{22} + \sigma_{12} - \sigma_{22}\rho_R^{(2)} - \sigma_{21}\rho_R^{(1)} - \sigma_{12}\rho_R^{(2)} - \sigma_{11}\rho_R^{(1)} & m + \sigma_{11}\rho_R^{(1)} + \sigma_{12}\rho_R^{(2)} & \sigma_{21}\rho_R^{(1)} - \sigma_{12} - m - \sigma_{22} + \sigma_{22}\rho_R^{(2)} \end{pmatrix} \tag{85}$$

C Details of the Proof of Theorem 4.1

C.1 Bulk Process

To solve (34) it is useful to rewrite the system by using the following variables, that are made by sums of three non diagonal rates:

$$y_1 = \sum_{\beta=0}^{2} \Gamma_{10}^{\beta 1} \quad y_2 = \sum_{\beta=0}^{2} \Gamma_{00}^{\beta 1} \quad y_3 = \sum_{\beta=0}^{2} \Gamma_{01}^{1\beta} \quad y_4 = \sum_{\beta=0}^{2} \Gamma_{00}^{1\beta} \quad y_5 = \sum_{\beta=0}^{2} \Gamma_{10}^{0\beta} \quad y_6 = \sum_{\beta=0}^{2} \Gamma_{10}^{2\beta}$$

$$y_7 = \sum_{\beta=0}^{2} \Gamma_{01}^{\beta 0} \quad y_8 = \sum_{\beta=0}^{2} \Gamma_{01}^{\beta 2} \quad y_9 = \sum_{\beta=0}^{2} \Gamma_{20}^{\beta 1} \quad y_{10} = \sum_{\beta=0}^{2} \Gamma_{02}^{1\beta} \quad y_{11} = \sum_{\beta=0}^{2} \Gamma_{02}^{\beta 1} \quad y_{12} = \sum_{\beta=0}^{2} \Gamma_{20}^{1\beta}$$

$$y_{13} = \sum_{\beta=0}^{2} \Gamma_{20}^{\beta 2} \quad y_{14} = \sum_{\beta=0}^{2} \Gamma_{00}^{\beta 2} \quad y_{15} = \sum_{\beta=0}^{2} \Gamma_{02}^{2\beta} \quad y_{16} = \sum_{\beta=0}^{2} \Gamma_{00}^{2\beta} \quad y_{17} = \sum_{\beta=0}^{2} \Gamma_{20}^{0\beta} \quad y_{18} = \sum_{\beta=0}^{2} \Gamma_{02}^{\beta 0}$$

$$y_{19} = \sum_{\beta=0}^{2} \Gamma_{10}^{\beta 2} \quad y_{20} = \sum_{\beta=0}^{2} \Gamma_{01}^{2\beta} \quad y_{21} = \sum_{\beta=0}^{2} \Gamma_{11}^{\beta 0} \quad y_{22} = \sum_{\beta=0}^{2} \Gamma_{21}^{\beta 0} \quad y_{23} = \sum_{\beta=0}^{2} \Gamma_{22}^{\beta 1} \quad y_{24} = \sum_{\beta=0}^{2} \Gamma_{11}^{0\beta}$$

$$y_{25} = \sum_{\beta=0}^{2} \Gamma_{12}^{0\beta} \quad y_{26} = \sum_{\beta=0}^{2} \Gamma_{12}^{\beta 1} \quad y_{27} = \sum_{\beta=0}^{2} \Gamma_{21}^{1\beta} \quad y_{28} = \sum_{\beta=0}^{2} \Gamma_{22}^{1\beta} \quad y_{29} = \sum_{\beta=0}^{2} \Gamma_{11}^{\beta 2} \quad y_{30} = \sum_{\beta=0}^{2} \Gamma_{12}^{\beta 0}$$

$$y_{31} = \sum_{\beta=0}^{2} \Gamma_{21}^{\beta 2} \quad y_{32} = \sum_{\beta=0}^{2} \Gamma_{22}^{\beta 0} \quad y_{33} = \sum_{\beta=0}^{2} \Gamma_{11}^{2\beta} \quad y_{34} = \sum_{\beta=0}^{2} \Gamma_{12}^{2\beta} \quad y_{35} = \sum_{\beta=0}^{2} \Gamma_{21}^{0\beta} \quad y_{36} = \sum_{\beta=0}^{2} \Gamma_{22}^{0\beta}$$

Let us introduce the following:

- *unknown vector*: $\mathbf{y} \in \mathbb{R}_{+}^{36}$

$$\mathbf{y} = (y_i)_{i=1,\ldots 36}$$

- *known term*: $\mathbf{b} \in \mathbb{R}^{30}$ (that is exactly the one in (34))

$$\mathbf{b} = (\sigma_{11}, \sigma_{11}, -2\sigma_{11} - \Upsilon, \sigma_{12}, \sigma_{12}, -2\sigma_{12} + \Upsilon, \sigma_{22}, \sigma_{22}, -2\sigma_{22} - \Upsilon, \sigma_{21}, \sigma_{21},$$
$$-2\sigma_{21} + \Upsilon, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T$$

- *coefficient matrix*: $\Xi \in \mathbb{R}^{30\times 36}$ (that is full rank)

By using the above vectors and matrix, the system (34) can be rewritten as

$$\Xi \mathbf{y} = \mathbf{b}. \tag{86}$$

The systems (34) and (86) are two ways of writing the conditions (31), (32), (33). By consequence, there exists an other full rank matrix, say $\Lambda \in \mathbb{R}^{36\times 72}$, that allows to retrieve a 36 parameter family of solutions of (34) once we know the one of (86) as follows

$$\Lambda \mathbf{u} = \mathbf{y}. \tag{87}$$

We first solve (86) and then we retrieve the specific solution (84) of (34), by solving (87) with some specific choices of the 36 parameters.

Solution of (86): the under-determination order is 6 and thus 6 components of the vector $\mathbf{y}$ are, actually, free parameters. Without any constraint (86) would have a 6 parameter family of solutions. However, the non-negativity of the solution (the y_i are sums of transition rates) will reduce the dependence on just two free parameters.

Indeed, by direct computations and by recalling that the variables $\{y_j\}_{j=1,\ldots 36}$ must be non-negative we find the following 12 unknowns by using just 10 equations, namely:

$$y_1 - y_2 = \sigma_{11} \quad y_3 - y_4 = \sigma_{11} \quad y_9 - y_2 = \sigma_{12} \quad y_{10} - y_4 = \sigma_{12} \quad y_{13} - y_{14} = \sigma_{22}$$
$$y_{15} - y_{16} = \sigma_{22} \quad y_{19} - y_{14} = \sigma_{21} \quad y_{20} - y_{16} = \sigma_{21} \quad y_2 + y_{14} = 0 \quad y_4 + y_{16} = 0$$

that are solved if and only if

$$y_2 = y_4 = y_{14} = y_{16} = 0 \qquad y_1 = y_3 = \sigma_{11} \qquad y_{19} = y_{20} = \sigma_{21}$$
$$y_9 = y_{10} = \sigma_{12} \qquad y_{13} = y_{15} = \sigma_{22}.$$

By the non negativeness of the above y_j, it follows that

$$\sigma_{11}, \sigma_{12}, \sigma_{21}, \sigma_{22} \geq 0. \tag{88}$$

Now, it remains to solve a system with 20 equations and 24 unknowns. By introducing as parameters $(y_7, y_8, y_{11}, y_{17}) := (g, h, m, s)$, this 20×24 system becomes a 20×20 parametric system. This last one has the following explicit parametric solution:

$$\begin{aligned}
&(y_5,\ y_6,\ y_{12},\ y_{18},\ y_{21},\ y_{22},\ y_{23},\ y_{24},\ y_{25},\ y_{26},\ y_{27},\\
&\quad y_{28},\ y_{29},\ y_{30},\ y_{31},\ y_{32},\ y_{33},\ y_{34},\ y_{35},\ y_{36})\\
&= (2\sigma_{11} + 2\sigma_{21} - g,\ \Upsilon - 2\sigma_{21} - h,\ \Upsilon - 2\sigma_{12} - m,\ 2\sigma_{12} + 2\sigma_{22} - s,\\
&\quad g - \sigma_{21} - \sigma_{11},\ g - \sigma_{22} - \sigma_{12},\ \sigma_{12} + m,\\
&\quad \sigma_{11} + \sigma_{21} - g, 2\sigma_{11} - \sigma_{12} + 2\sigma_{21} - \sigma_{22} - g,\ \sigma_{11} + m,\\
&\quad \sigma_{11} - 2\sigma_{12} + \sigma - m, \Upsilon - \sigma_{12} - m,\ \sigma_{21} + h,\\
&\quad 2\sigma_{12} - \sigma_{11} - \sigma_{21} + 2\sigma_{22} - s,\ \sigma_{22} + h,\ \sigma_{12} + \sigma_{22} - s,\\
&\quad \Upsilon - \sigma_{21} - h,\ \sigma_{22} - 2\sigma_{21} + \Upsilon - h, s - \sigma_{21} - \sigma_{11},\\
&\quad s - \sigma_{22} - \sigma_{12})\,.
\end{aligned} \tag{89}$$

Since all the y_i are sums of non negative transition rates, we impose that the components of (89) are non negative. This is true if and only if:

$$s = \sigma_{11} + \sigma_{21} \quad g = \sigma_{11} + \sigma_{21} \tag{90}$$

and

$$\Upsilon, h, m \geq 0 \qquad \sigma_{12} \leq \frac{\Upsilon - m}{2} \qquad \sigma_{21} \leq \frac{\Upsilon - h}{2} \qquad \sigma_{11} + \sigma_{21} = \sigma_{12} + \sigma_{22}. \tag{91}$$

Since (90) fixes the value of two of the four parameters, the non negative solution only depends on h, m. Putting together (88) and (91) we obtain (40). Finally, this explicit non-negative solution of (86) is

$$\begin{aligned}
\mathbf{y} = (&\sigma_{11},\ 0,\ \sigma_{11}\ 0,\ \sigma_{11} + \sigma_{21},\ \Upsilon - 2\sigma_{21} - h,\ \sigma_{11} + \sigma_{21},\\
&h,\ \sigma_{12},\ \sigma_{12},\ m,\ \Upsilon - 2\sigma_{12} - m,\\
&\sigma_{11} - \sigma_{12} + \sigma_{21},\ 0,\ \sigma_{11} - \sigma_{12} + \sigma_{21},\ 0,\ \sigma_{11} + \sigma_{21},\ \sigma_{11}\\
&+ \sigma_{21}\sigma_{21},\ \sigma_{21},\ 0,\ 0,\ \sigma_{12} + m,\ 0,\ 0,\ \sigma_{11} + m,\\
&\sigma_{11} - 2\sigma_{12} + \Upsilon - m,\ \Upsilon - \sigma_{12} - m,\\
&\sigma_{21} + h,\ 0,\ \sigma_{11} - \sigma_{12} + \sigma_{21} + h,\ 0,\ \Upsilon - \sigma_{21} - h,\\
&\sigma_{11} - \sigma_{12} - \sigma_{21} + \Upsilon - h,\ 0,\ 0)
\end{aligned} \tag{92}$$

Solution of (34): from (92) we know the explicit solution of (86). To find the solution of (34), we solve (87). This last system is full rank. It has 72 unknowns in 36 equations, thus the order of under-determination is 36. We must look for non-negative solution. To remove the under-determination, and produce examples (84) we impose the following conditions:

i The matrix associated to the generator has the greater number of zeros;
ii Fix the following rates:

$$\Gamma_{12}^{21} = \sigma_{11} \quad \Gamma_{21}^{12} = \sigma_{22} \quad \Gamma_{11}^{22} = \sigma_{21} \quad \Gamma_{22}^{11} = \sigma_{12}. \tag{93}$$

With the above two requests, the solution of (87) is unique (for fixed parameters h, m and for fixed diffusivity matrix and reaction constant) and the bulk generator takes the form (84). Indeed, by considering (92) we have:

- The row $\Gamma_{00}^{\alpha,\beta}$ has all the elements are zero;
- The row $\Gamma_{01}^{\alpha,\beta}$ is found by solving

$$\Gamma_{01}^{10} + \Gamma_{01}^{11} + \Gamma_{01}^{12} = \sigma_{11} \qquad \Gamma_{01}^{00} + \Gamma_{01}^{10} + \Gamma_{01}^{20} = \sigma_{11} + \sigma_{21}$$
$$\Gamma_{01}^{02} + \Gamma_{01}^{12} + \Gamma_{01}^{22} = h \qquad \Gamma_{01}^{20} + \Gamma_{01}^{21} + \Gamma_{01}^{22} = \sigma_{21}.$$

  By the conditions i and ii previously required, we obtain $\Gamma_{01}^{10} = \sigma_{11}, \Gamma_{01}^{20} = \sigma_{12}, \Gamma_{01}^{02} = h$ and all the other off-diagonal rates are equal to zero. By similar arguments, also the rows $\Gamma_{02}^{\alpha\beta}, \Gamma_{10}^{\alpha\beta}, \Gamma_{20}^{\alpha\beta}$ are determined.
- The row $\Gamma_{11}^{\alpha\beta}$ is found by solving:

$$\Gamma_{11}^{02} + \Gamma_{11}^{12} + \Gamma_{11}^{22} = \sigma_{21} + h \qquad \Gamma_{11}^{20} + \Gamma_{11}^{21} + \Gamma_{11}^{22} = \Upsilon - \sigma_{21} - h$$
$$\Gamma_{11}^{00} + \Gamma_{11}^{10} + \Gamma_{11}^{20} = 0 \qquad \Gamma_{11}^{00} + \Gamma_{11}^{01} + \Gamma_{11}^{02} = 0.$$

  By the conditions i and ii previously required we obtain $\Gamma_{11}^{22} = \sigma_{21}, \Gamma_{11}^{12} = h, \Gamma_{11}^{21} = \Upsilon - 2\sigma_{21} - h$ and all the other off-diagonal rates are equal to zero. By similar arguments, also the rows $\Gamma_{12}^{\alpha\beta}, \Gamma_{21}^{\alpha\beta}, \Gamma_{22}^{\alpha\beta}$ are determined.

We observe that, when $h = m = 0$ (84) do coincide with the non negative least square solution (see [37]) of (87). (42) is recovered from (84) when $\sigma_{21} = \sigma_{12}$, $\sigma_{22} = \sigma_{11}$ and $h = m$ in (84).

C.2 Boundary Processes

Once the bulk is known, the conditions for the boundaries form two determined systems of linear algebraic equations. We solve explicitly only the left boundary; the solution of the right one is very similar.

Left boundary: recalling the definitions of B_1 and C_2, we have the following

$$B_1^{11} = -y_5 - y_6 - y_4 \quad B_1^{12} = y_{12} - y_4 \quad B_1^{21} = y_6 - y_{16} \quad B_1^{22} = -y_{17} - y_{12} - y_{16}$$
$$C_2^{11} = -y_7 - h - y_2 \quad C_2^{12} = m - y_2 \quad C_2^{21} = h - y_{14} \quad C_2^{22} = -y_{18} - m - y_{14};$$

by consequence system (37) is rewritten as:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 & -1 \end{pmatrix} \begin{pmatrix} W_0^1(1) \\ W_0^2(1) \\ W_1^0(1) \\ W_1^2(1) \\ W_2^0(1) \\ W_2^1(1) \end{pmatrix} = \begin{pmatrix} \sigma_{11}\rho_L^{(1)} + \sigma_{12}\rho_L^{(2)} \\ -\sigma_{11} - \sigma_{21} - h \\ m \\ \sigma_{21}\rho_L^{(1)} + \sigma_{22}\rho_L^{(2)} \\ h \\ -\sigma_{22} - \sigma_{12} - m \end{pmatrix}.$$

The coefficient matrix of the above system has full rank; thus there exists a unique solution. Recalling the definition of $W^{\alpha}_{\gamma}(1)$ we obtain (83). As a consequence of (40), and in particular $\sigma_{11} + \sigma_{21} = \sigma_{12} + \sigma_{22}$, this generator has non negative non-diagonal transition rates if

$$0 \leq \rho^{(1)}_L + \rho^{(2)}_L \leq 1. \tag{94}$$

(94) is always true since we assumed that the sum of the densities of the two species in the reservoir is at most one.

Right boundary: by similar arguments we solve (38) and we obtain the right boundary, i.e. (85). This matrix has non-negative off-diagonal rates if:

$$0 \leq \rho^{(1)}_R + \rho^{(2)}_R \leq 1. \tag{95}$$

(95) is always true since we assumed that the sum of the densities in the reservoir is at most one.

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