Multispecies reaction-diffusion systems

A. Aghamohammadi,[1,2,*] A. H. Fatollahi,[2,3,†] M. Khorrami,[2,3,‡] and A. Shariati[2,3,§]
[1]*Department of Physics, Alzahra University, Tehran 19834, Iran*
[2]*Institute for Studies in Theoretical Physics and Mathematics, P.O. Box 5531, Tehran 19395, Iran*
[3]*Institute for Advanced Studies in Basic Sciences, P.O. Box 159, Gava Zang, Zanjan 45195, Iran*
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Multispecies reaction-diffusion systems, for which the time evolution equations of correlation functions become a closed set, are considered. A formal solution for the average densities is found. Some special interactions and the exact time dependence of the average densities in these cases are also studied. For the general case, the large-time behavior of the average densities has also been obtained.

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I. INTRODUCTION

In recent years, reaction-diffusion systems have been studied by many people. As mean field techniques generally do not give correct results for low-dimensional systems, people are motivated to study stochastic models in low dimensions. Moreover, solving one-dimensional systems should in principle be easier. Exact results for some models in a one-dimensional lattice have been obtained, for example, in [1–10].

Different methods have been used to study these models, including analytical and asymptotic methods, mean field methods, and large-scale numerical methods. Systems with more than one species have also been studied [11–22]. Most of the arguments are based on simulation results. There are, however, some exact results as well ([18,20,22], for example).

In [23], a ten-parameter family of stochastic models has been studied. In these models, the k-point equal time correlation functions $\langle n_i n_j \ldots n_k \rangle$ satisfy linear differential equations involving no higher-order correlations. These linear equations for the average density $\langle n_i \rangle$ have been solved, but this set of equations cannot be solved easily for higher-order correlation functions. We have generalized the same idea to multispecies models. We have considered general reaction-diffusion processes of multiple species in one dimension with two-site interaction. We have obtained the conditions the Hamiltonian should satisfy in order to give rise to a closed set of time evolution equations for the correlation functions. The set of equations for average densities can be written in terms of four matrices. The time evolution equations for more-point functions, besides these four matrices, generally depend explicitly on the elements of the Hamiltonian, and generally cannot be solved easily. These matrices are not determined uniquely from the Hamiltonian: there is a kind of gauge transformation one can apply on them which, of course, does not change the evolution equation. A formal solution for average densities of different species is found. For some special choices of the four matrices we also give the explicit form of the interactions and the exact time dependence of the average densities. At the end, we study the large-time behavior of the average densities of different species for the general case.

II. A BRIEF REVIEW OF LINEAR STOCHASTIC SYSTEMS

To fix the notation used in this article, here we briefly review the already well known formalism of linear stochastic systems. The master equation for $P(\sigma,t)$ is

$$\frac{\partial}{\partial t}P(\sigma,t)=\sum_{\tau\neq\sigma}\left[\omega(\tau\rightarrow\sigma)P(\tau,t)-\omega(\sigma\rightarrow\tau)P(\sigma,t)\right], \tag{1}$$

where $\omega(\tau\rightarrow\sigma)$ is the transition rate from the configuration τ to σ. Introducing the state vector

$$|P\rangle=\sum_{\sigma}P(\sigma,t)|\sigma\rangle, \tag{2}$$

where the summation runs over all possible states of the system, one can write the above equation in the form

$$\frac{d}{dt}|P\rangle=\mathcal{H}|P\rangle, \tag{3}$$

where the matrix elements of $\mathcal{H}$ are

$$\begin{aligned}\langle\sigma|\mathcal{H}|\tau\rangle&=\omega(\tau\rightarrow\sigma),\quad \tau\neq\sigma,\\ \langle\sigma|\mathcal{H}|\sigma\rangle&=-\sum_{\tau\neq\sigma}\omega(\sigma\rightarrow\tau).\end{aligned} \tag{4}$$

The basis $\{\langle\sigma|\}$ is dual to $\{|\sigma\rangle\}$, that is,

$$\langle\sigma|\tau\rangle=\delta_{\sigma\tau}. \tag{5}$$

The operator $\mathcal{H}$ is called a Hamiltonian, and it is not necessarily Hermitian. Conservation of probability,

$$\sum_{\sigma}P(\sigma,t)=1, \tag{6}$$

*Email address: mohamadi@theory.ipm.ac.ir
†Email address: fath@iasbs.ac.ir
‡Email address: mamwad@iasbs.ac.ir
§Email address: shahram@iasbs.ac.ir

shows that

$$\langle S|\mathcal{H}=0, \tag{7}$$

where

$$\langle S|=\sum_{\beta}\langle \beta|. \tag{8}$$

So the sum of each column of $\mathcal{H}$, as a matrix, should be zero. As $\langle S|$ is a left eigenvector of $\mathcal{H}$ with zero eigenvalue, $\mathcal{H}$ has at least one right eigenvector with zero eigenvalue. This state corresponds to the steady state distribution of the system and it does not evolve in time. If the zero eigenvalue is degenerate, the steady state is not unique. The transition rates are non-negative, so the off-diagonal elements of the matrix $\mathcal{H}$ are non-negative. Therefore, if a matrix $\mathcal{H}$ has the properties

$$\begin{aligned}\langle S|\mathcal{H}&=0,\\ \langle \sigma|\mathcal{H}|\tau\rangle&\geqslant 0,\end{aligned} \tag{9}$$

then it can be considered as the generator of a stochastic process. It can be proved that the real part of the eigenvalues of any matrix with the above conditions is less than or equal to zero.

The dynamics of the state vectors (3) is given by

$$|P(t)\rangle=\exp(t\mathcal{H})|P(0)\rangle, \tag{10}$$

and the expectation value of an observable $\mathcal{O}$ is

$$\langle \mathcal{O}\rangle(t)=\sum_{\sigma}\mathcal{O}(\sigma)P(\sigma,t)=\langle S|\mathcal{O}\exp(t\mathcal{H})|P(0)\rangle. \tag{11}$$

III. MODELS LEADING TO A CLOSED SET OF EVOLUTION EQUATIONS

The models that we address are multispecies reaction-diffusion models. That is, each site is a vacancy or has one particle. There are several kinds of particle, but at any time at most one kind can be present at each site. Suppose the interaction is between nearest neighbors, and the system is translationally invariant,

$$\mathcal{H}=\sum_{i=1}^{L}H_{i,i+1}. \tag{12}$$

The number of sites is L and the number of possible states in a site is N; different states of each site are denoted by A_α, $\alpha=1,\ldots N$, where one of the states is a vacancy. Introducing n_i^α as the number operator of the A_α particle in the site i, we have

$$\sum_{\alpha=1}^{N}n_i^\alpha=1. \tag{13}$$

The average number density of the particle A_α in the site i at the time t is

$$\langle n_i^\alpha\rangle=\langle S|n_i^\alpha|P(t)\rangle, \tag{14}$$

where $|P(t)\rangle:=\exp(t\mathcal{H})|P(0)\rangle$ represents the state of the system at the time t,

$$\langle S|=\underbrace{\langle s|\otimes\ldots\otimes\langle s|}_{L}, \tag{15}$$

and

$$\langle s|:=(\underbrace{11\ldots1}_{N}). \tag{16}$$

So the time evolution of $\langle n_i^\alpha\rangle$ is given by

$$\frac{d}{dt}\langle n_i^\alpha\rangle=\langle S|n_i^\alpha\mathcal{H}|P(t)\rangle. \tag{17}$$

The only terms of the Hamiltonian $\mathcal{H}$ that are relevant in the above equation are $H_{i,i+1}$ and $H_{i-1,i}$. The result of acting any matrix Q on the ket $\langle s|$ is equivalent to acting the diagonal matrix $\tilde{Q}$ on the same ket, provided each diagonal element of the matrix $\tilde{Q}$ is the sum of all elements of the corresponding column in the matrix Q. So the actions of $(1\otimes n^\alpha)H$ and $(n^\alpha\otimes 1)H$ on $\langle s|\otimes\langle s|$ are equivalent to the action of two diagonal matrices on $\langle s|\otimes\langle s|$. We use the notation $\sim$ for the equivalent action on $\langle s|\otimes\langle s|$:

$$\begin{aligned}(1\otimes n^\alpha)H&\sim\sum_{\beta\gamma}\mathcal{A}_{\beta\gamma}^{\alpha}n^\beta\otimes n^\gamma,\\ (n^\alpha\otimes 1)H&\sim\sum_{\beta\gamma}\overline{\mathcal{A}}_{\beta\gamma}^{\alpha}n^\beta\otimes n^\gamma,\end{aligned} \tag{18}$$

where $\mathcal{A}_{\beta\gamma}^{\alpha}$ and $\overline{\mathcal{A}}_{\beta\gamma}^{\alpha}$ are

$$\begin{aligned}\mathcal{A}_{\beta\gamma}^{\alpha}&:=\sum_{\lambda}H_{\beta\gamma}^{\lambda\alpha},\\ \overline{\mathcal{A}}_{\beta\gamma}^{\alpha}&:=\sum_{\lambda}H_{\beta\gamma}^{\alpha\lambda}.\end{aligned} \tag{19}$$

Then, Eq. (17) takes the form

$$\langle \dot{n}_i^\alpha\rangle=\sum_{\beta\gamma}\mathcal{A}_{\beta\gamma}^{\alpha}\langle n_{i-1}^\beta n_i^\gamma\rangle+\overline{\mathcal{A}}_{\beta\gamma}^{\alpha}\langle n_i^\beta n_{i+1}^\gamma\rangle. \tag{20}$$

Generally, in the time evolution equation of $\langle n^\alpha\rangle$ the two-point functions $\langle n^\beta n^\gamma\rangle$ appear. Using Eq. (13), one can see that if and only if $\mathcal{A}$ and $\overline{\mathcal{A}}$ satisfy the following equations, then the right hand side of Eq. (20) can be expressed in terms of only one-point functions:

$$\begin{aligned}\mathcal{A}_{\beta\gamma}^{\alpha}+\mathcal{A}_{NN}^{\alpha}-\mathcal{A}_{N\gamma}^{\alpha}-\mathcal{A}_{\beta N}^{\alpha}&=0,\\ \overline{\mathcal{A}}_{\beta\gamma}^{\alpha}+\overline{\mathcal{A}}_{NN}^{\alpha}-\overline{\mathcal{A}}_{N\gamma}^{\alpha}-\overline{\mathcal{A}}_{\beta N}^{\alpha}&=0.\end{aligned} \tag{21}$$

These equations give $2(N-1)^3$ constraints on the Hamiltonian, so adding the condition of stochasticity of H, we have $2(N-1)^3+N^2$ relations between the elements of H. The constraints (21) mean

$$\mathcal{A}_{\beta\gamma}^{\alpha}=C_\beta^\alpha-B_\gamma^\alpha,$$

$$\bar{\mathcal{A}}^{\alpha}_{\beta\gamma} = -\bar{B}^{\alpha}_{\beta} + \bar{D}^{\alpha}_{\gamma}. \tag{22}$$

So Eq. (17) takes the form

$$\langle \dot{n}_i^{\alpha} \rangle = \sum_{\beta=1}^{N} [-(B^{\alpha}_{\beta} + \bar{B}^{\alpha}_{\beta})\langle n_i^{\beta}\rangle + C^{\alpha}_{\beta}\langle n_{i-1}^{\beta}\rangle + \bar{D}^{\alpha}_{\beta}\langle n_{i+1}^{\beta}\rangle]. \tag{23}$$

In the simplest case, of one species, each site is vacant or occupied by only one kind of particles. Then the matrices B, C, $\bar{B}$, and $\bar{D}$ are two dimensional. Using Eq. (13), the equation for $\langle \dot{n}_i^1 \rangle$ is

$$\begin{aligned}\langle \dot{n}_i^1 \rangle = {} & (-B_1^1 - \bar{B}_1^1 + B_2^1 + \bar{B}_2^1)\langle n_i^1\rangle + (C_1^1 - C_2^1)\langle n_{i-1}^1\rangle \\ & + (\bar{D}_1^1 - \bar{D}_2^1)\langle n_{i+1}^1\rangle + (-B_2^1 - \bar{B}_2^1 + C_2^1 + \bar{D}_2^1).\end{aligned} \tag{24}$$

This is a linear difference equation of the kind obtained in [23], and its solution can be expressed in terms of modified Bessel functions.

The time evolution equation for two-point functions can also be obtained:

$$\begin{aligned}\frac{d}{dt}\langle n_i^{\alpha} n_j^{\beta}\rangle = \sum_{\gamma}^{N} {} & [-(B^{\alpha}_{\gamma} + \bar{B}^{\alpha}_{\gamma})\langle n_i^{\gamma} n_j^{\beta}\rangle + C^{\alpha}_{\gamma}\langle n_{i-1}^{\gamma} n_j^{\beta}\rangle \\ & + \bar{D}^{\alpha}_{\gamma}\langle n_{i+1}^{\gamma} n_j^{\beta}\rangle - (B^{\beta}_{\gamma} + \bar{B}^{\beta}_{\gamma})\langle n_i^{\alpha} n_j^{\gamma}\rangle \\ & + C^{\beta}_{\gamma}\langle n_i^{\alpha} n_{j-1}^{\gamma}\rangle + \bar{D}^{\beta}_{\gamma}\langle n_i^{\alpha} n_{j+1}^{\gamma}\rangle], \quad |i-j|>1,\end{aligned} \tag{25}$$

$$\begin{aligned}\frac{d}{dt}\langle n_i^{\alpha} n_{i+1}^{\beta}\rangle = \sum_{\gamma}^{N} {} & [-B^{\alpha}_{\gamma}\langle n_i^{\gamma} n_{i+1}^{\beta}\rangle - \bar{B}^{\beta}_{\gamma}\langle n_i^{\alpha} n_{i+1}^{\gamma}\rangle \\ & + C^{\alpha}_{\gamma}\langle n_{i-1}^{\gamma} n_{i+1}^{\beta}\rangle + \bar{D}^{\beta}_{\gamma}\langle n_i^{\alpha} n_{i+2}^{\gamma}\rangle] \\ & + \sum_{\gamma\lambda} H^{\alpha\beta}_{\gamma\lambda}\langle n_i^{\gamma} n_{i+1}^{\lambda}\rangle.\end{aligned} \tag{26}$$

For more-point functions, one can deduce similar results. In fact, it is easy to show that if the evolution equations of one-point functions are closed, the evolution equations of n-point functions contain only n- and fewer-point functions. However, generally these sets of equations cannot be solved easily.

IV. EQUIVALENT HAMILTONIANS REGARDING ONE-POINT FUNCTIONS AND GAUGE TRANSFORMATIONS

Knowing B, C, $\bar{B}$, and $\bar{D}$ does not determine the Hamiltonian uniquely, but as is seen from Eq. (23) the time evolution of one-point functions depends only on B, C, $\bar{B}$, and $\bar{D}$. The two- and more-point functions depend explicitly on the elements of H. So different Hamiltonians may give the same evolution for $\langle n_i^{\alpha}\rangle$. Take two Hamiltonians H and H'. Defining

$$R := H - H', \tag{27}$$

if

$$\sum_{\alpha} R^{\alpha\beta}_{\gamma\lambda} = \sum_{\beta} R^{\alpha\beta}_{\gamma\lambda} = 0, \tag{28}$$

these two Hamiltonians give rise to the same $\mathcal{A}$ and $\bar{\mathcal{A}}$. Regarding one-point functions $\langle n_i^{\alpha}\rangle$, these models are the same. So we call these models equivalent regarding one-point functions.

However, $\mathcal{A}$ and $\bar{\mathcal{A}}$ do not determine B, C, $\bar{B}$, and $\bar{D}$ uniquely. The stochastic condition

$$\sum_{\alpha\beta} H^{\alpha\beta}_{\gamma\lambda} = 0 \tag{29}$$

results in some constraints on B, C, $\bar{B}$, and $\bar{D}$:

$$\begin{aligned}\sum_{\alpha} (C^{\alpha}_{\beta} - B^{\alpha}_{\gamma}) = 0, \\ \sum_{\alpha} (-\bar{B}^{\alpha}_{\beta} + \bar{D}^{\alpha}_{\gamma}) = 0.\end{aligned} \tag{30}$$

Thus the sum of all elements of any column of $B(C)$ should be the same:

$$\sum_{\alpha} C^{\alpha}_{\beta} = \sum_{\alpha} B^{\alpha}_{\beta} = f. \tag{31}$$

Then the state $\langle s|$ is the left eigenvector of B and C, with the same eigenvalue f. $\bar{B}$ and $\bar{D}$ also have the same property, of course with different eigenvalue g.

Changing B and C according to the *gauge* transformation

$$\begin{aligned}C^{\alpha}_{\beta} \to C'^{\alpha}_{\beta} = C^{\alpha}_{\beta} - f^{\alpha} \quad \text{or} \quad C' = C - |f\rangle\langle s|, \\ B^{\alpha}_{\beta} \to B'^{\alpha}_{\beta} = B^{\alpha}_{\beta} - f^{\alpha} \quad \text{or} \quad B' = B - |f\rangle\langle s|\end{aligned} \tag{32}$$

does not change $\mathcal{A}$. With a suitable choice of f^{α},

$$\sum_{\alpha} f^{\alpha} = f, \tag{33}$$

the sum of the elements of any column of B or C can be set to zero. In this gauge, the eigenvalues of B and C for the eigenvector $\langle s|$ will be zero.

V. ONE-POINT FUNCTIONS

To solve Eq. (23), we introduce the vector $\mathcal{N}_k$:

$$\mathcal{N}_k := \begin{pmatrix} \langle n_k^1\rangle \\ \langle n_k^2\rangle \\ \cdot \\ \cdot \\ \cdot \\ \langle n_k^N\rangle \end{pmatrix}. \tag{34}$$

Equation (23) can then be written as

$$\dot{\mathcal{N}}_k = -(B+\overline{B})\mathcal{N}_k + C\mathcal{N}_{k-1} + \overline{D}\mathcal{N}_{k+1}. \tag{35}$$

Introducing the generating function $G(z,t)$,

$$G(z,t) = \sum_{-\infty}^{\infty} \mathcal{N}_k(t) z^k, \tag{36}$$

one arrives at

$$\dot{G}(z,t) = [-(B+\overline{B}) + zC + z^{-1}\overline{D}]G(z,t), \tag{37}$$

the solution to which is

$$G(z,t) = \exp\{t[-(B+\overline{B}) + zC + z^{-1}\overline{D}]\}G(z,0). \tag{38}$$

The $\mathcal{N}_k(t)$'s are the coefficients of the Laurent expansion of $G(z,t)$, so

$$\mathcal{N}_k(t) = \frac{1}{2\pi i} \sum_{m=-\infty}^{\infty} \oint dz z^{m-k-1} \exp\{t[-(B+\overline{B}) + zC + z^{-1}\overline{D}]\}\mathcal{N}_m(0). \tag{39}$$

This is the formal solution of the problem, which is of the form

$$\mathcal{N}_k(t) = \sum_m \Gamma_{km}(t)\mathcal{N}_m(0). \tag{40}$$

A. Some special cases

We now consider special choices for B, C, $\overline{B}$, and $\overline{D}$.

1. The matrices B, C, $\overline{B}$, and $\overline{D}$ are two dimensional (the single-species case)

We can use the gauge transformation to make $\langle s|$ the simultaneous null left eigenvector of B, C, $\overline{B}$, and $\overline{D}$. In this gauge, one has

$$\begin{aligned} B &= |u\rangle\langle b|, \\ C &= |u\rangle\langle c|, \\ \overline{B} &= |u\rangle\langle \overline{b}|, \\ D &= |u\rangle\langle d|, \end{aligned} \tag{41}$$

where

$$|u\rangle := \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{42}$$

This means that it is orthogonal to $\langle s|$ and is a simultaneous right eigenvector of B, C, $\overline{B}$, and $\overline{D}$. Using Eq. (41), one can easily calculate the exponential in Eq. (39):

$$\exp\{t[-(B+\overline{B}) + zC + z^{-1}\overline{D}]\} = 1 + \frac{e^{tg(z)}-1}{g(z)}|u\rangle\langle g(z)|, \tag{43}$$

where

$$\langle g(z)| := -\langle b| - \langle \overline{b}| + z\langle c| + z^{-1}\langle \overline{d}| \tag{44}$$

and

$$g(z) := \langle g(z)|u\rangle. \tag{45}$$

Now take $\langle v|$ and $|w\rangle$ to be the left eigenvector of $-B-\overline{B}+C+\overline{D}$ dual to $|u\rangle$ and the right eigenvector of $-B-\overline{B}+C+\overline{D}$ dual to $\langle s|$, respectively. One can normalize these, so that

$$\begin{aligned} \langle v|u\rangle &= 1, \\ \langle s|w\rangle &= 1. \end{aligned} \tag{46}$$

Of course, $\langle v|$ is orthogonal to $|w\rangle$. Then,

$$\begin{aligned} &\exp\{t[-(B+\overline{B}) + zC + z^{-1}\overline{D}]\} \\ &\quad = e^{tg(z)}|u\rangle\langle v| + |w\rangle\langle s| + \langle g(z)|w\rangle \\ &\qquad \times \frac{e^{tg(z)}-1}{g(z)}|u\rangle\langle s|. \end{aligned} \tag{47}$$

Acting this on $\mathcal{N}_m(0)$, and noting that

$$\langle s|N_m(0) = 1, \tag{48}$$

it is seen that

$$\begin{aligned} N_k(t) &= |w\rangle\langle s|N_k(0) + \frac{1}{2\pi i}\sum_{m=-\infty}^{\infty} \oint dz z^{m-k-1} \\ &\quad \times e^{tg(z)}|u\rangle\langle v|\mathcal{N}_m(0) \\ &= |w\rangle + \frac{1}{2\pi i}\sum_{m=-\infty}^{\infty} \oint dz z^{m-k-1} e^{tg(z)}|u\rangle\langle v|\mathcal{N}_m(0), \end{aligned} \tag{49}$$

or

$$\langle v|N_k(t) = \frac{1}{2\pi i}\sum_{m=-\infty}^{\infty} \oint dz z^{m-k-1} e^{tg(z)}|u\rangle\langle v|\mathcal{N}_m(0). \tag{50}$$

This is equivalent to Eq. (24).

2. The case $C=pB$, $\overline{D}=q\overline{B}$

Using Eq. (22),

$$(1-p)\langle s|B = (1-q)\langle s|\overline{B} = 0, \tag{51}$$

means that $p=1$ or $\langle s|B=0$, and $q=1$ or $\langle s|\overline{B}=0$. If $\langle s|$ is not the left null eigenvector of B and $\overline{B}$, then $p=q=1$. So we will have $B=C$ and $\overline{D}=\overline{B}$. Now we use the definition of $\mathcal{A}$,

$$\mathcal{A}^{\alpha}_{\beta\gamma} = C^{\alpha}_{\beta} - C^{\alpha}_{\gamma} = \sum_{\lambda} H^{\lambda\alpha}_{\beta\gamma},$$

$$\mathcal{A}^{\alpha}_{\gamma\beta}=C^{\alpha}_{\gamma}-C^{\alpha}_{\beta}=\sum_{\lambda} H^{\lambda\alpha}_{\gamma\beta}. \tag{52}$$

For $\alpha\neq\beta$ and $\alpha\neq\gamma$, all the terms in the right hand side summations in the above equations are reaction rates and should be non-negative, but the sum of the left hand sides is zero. So

$$C^{\alpha}_{\beta}=C^{\alpha}_{\gamma}=f^{\alpha} \quad \text{for} \quad \gamma\neq\alpha\neq\beta. \tag{53}$$

All the elements of each row except the diagonal elements of C (or B) are the same. That is,

$$C=|f\rangle\langle s|+C', \tag{54}$$

where C' is some diagonal matrix. The fact that $|s\rangle$ is a left eigenvector of C shows that it should be a left eigenvector of C' as well, and this demands C' to be proportional to the unit matrix. One can make the same arguments for $\overline{B}$ and $\overline{D}$. So, after gauge transformation,

$$C=B=u\mathbf{1}, \quad \overline{D}=\overline{B}=v\mathbf{1}. \tag{55}$$

Although the time evolution of average densities can be written in terms of B, C, $\overline{B}$, and $\overline{D}$, the Hamiltonian H is not uniquely be determined by these matrices. There exist different Hamiltonians which are equivalent, regarding one-point functions:

$$\begin{aligned}\sum_{\lambda} H^{\lambda\alpha}_{\beta\gamma}&=\mathcal{A}^{\alpha}_{\beta\gamma}=u(\delta^{\alpha}_{\beta}-\delta^{\alpha}_{\gamma}),\\ \sum_{\lambda} H^{\alpha\lambda}_{\beta\gamma}&=\overline{\mathcal{A}}^{\alpha}_{\beta\gamma}=v(\delta^{\alpha}_{\gamma}-\delta^{\alpha}_{\beta}).\end{aligned} \tag{56}$$

All the elements of the $\beta\beta$ column of H are zero. For $\alpha\neq\beta$, the elements of H satisfy

$$\begin{aligned}\sum_{\lambda\neq\alpha,\beta} H^{\lambda\alpha}_{\alpha\beta}+H^{\alpha\alpha}_{\alpha\beta}+H^{\beta\alpha}_{\alpha\beta}&=u,\\ \sum_{\lambda\neq\alpha,\beta} H^{\lambda\beta}_{\alpha\beta}+H^{\alpha\beta}_{\alpha\beta}+H^{\beta\beta}_{\alpha\beta}&=-u,\\ \sum_{\lambda\neq\alpha,\beta} H^{\beta\lambda}_{\alpha\beta}+H^{\beta\alpha}_{\alpha\beta}+H^{\beta\beta}_{\alpha\beta}&=v,\\ \sum_{\lambda\neq\alpha,\beta} H^{\alpha\lambda}_{\alpha\beta}+H^{\alpha\alpha}_{\alpha\beta}+H^{\alpha\beta}_{\alpha\beta}&=-v.\end{aligned} \tag{57}$$

In general, these sets of equations have several solutions, but for the one-species case the reaction rates are the following:

$$A\varnothing\rightarrow\begin{cases}\varnothing A, & \Lambda_{12}\\ AA, & u-\Lambda_{12}\\ \varnothing\varnothing, & v-\Lambda_{12},\end{cases} \tag{58}$$

$$\varnothing A\rightarrow\begin{cases}A\varnothing, & \Lambda_{21}\\ AA, & v-\Lambda_{21}\\ \varnothing\varnothing, & u-\Lambda_{21}.\end{cases} \tag{59}$$

The above system, with no diffusion, was studied in [24]. There, the n-point functions were investigated. This solution can be generalized to the multispecies case. For $\alpha\neq\beta$,

$$A_{\alpha}A_{\beta}\rightarrow\begin{cases}A_{\beta}A_{a}, & \Lambda_{\alpha\beta},\alpha,\beta=1,\ldots,N\\ A_{\alpha}A_{\alpha}, & u-\Lambda_{\alpha\beta}\\ A_{\beta}A_{\beta}, & v-\Lambda_{\alpha\beta}.\end{cases} \tag{60}$$

The only constraint is the non-negativeness of the reaction rates:

$$u\geqslant\Lambda_{\alpha\beta}\geqslant 0, \quad v\geqslant\Lambda_{\alpha\beta}\geqslant 0. \tag{61}$$

This model has $N(N-1)+2$ free parameters. However, only the two parameters u and v appear in the time evolution equation of average densities:

$$\langle\dot{n}^{\alpha}_{i}\rangle=-(u+v)\langle n^{\alpha}_{i}\rangle+u\langle n^{\alpha}_{i-1}\rangle+v\langle n^{\alpha}_{i+1}\rangle. \tag{62}$$

As is seen, the dynamics of average densities of different particles decouple, and despite the complex interactions of the model, the $\langle\dot{n}^{\alpha}_{i}\rangle$'s can be easily calculated. But in the time evolution of two-point functions $\Lambda_{\alpha\beta}$'s appear as well. So, although models with different exchange rates ($\Lambda_{\alpha\beta}$) and the same initial conditions have the same average densities, their two-point functions generally are not the same.

3. B,$\overline{B}$,C,D commute

Generally, the gauge transformation do not preserve the commutation relation of B and C (and that of $\overline{B}$ and $\overline{D}$). But if B and C commute, there is a gauge transformation that leaves the transformed B and C commuting. If we choose $|f\rangle$ to be a right eigenvector of B and C dual to $\langle s|$, that is,

$$B|f\rangle=C|f\rangle=f|f\rangle, \tag{63}$$

then $B'\coloneqq B-|f\rangle\langle s|$ and $C'\coloneqq C-|f\rangle\langle s|$ commute. If

$$\langle s|f\rangle=f, \tag{64}$$

then $\langle s|$ times B' and C' will be zero. So, if B, C, $\overline{B}$, and $\overline{D}$ commute with each other, there exists a suitable gauge transformation that makes their eigenvalue corresponding to $\langle s|$ zero, while they remain commuting:

$$\langle s|B=\langle s|C=\langle s|\overline{B}=\langle s|\overline{D}=0. \tag{65}$$

Denote the matrix that simultaneously diagonalizes these four matrices by U, diagonalized matrices by primes, and their eigenvalues by b^{α}, c^{α}, $\overline{b}^{\alpha}$, and $\overline{d}^{\alpha}$, respectively. We have

$$\begin{aligned}\langle\Omega|B'=\langle\Omega|C'=\langle\Omega|\overline{B}'=\langle\Omega|\overline{D}'=0,\\ \langle\Omega|=\langle s|U.\end{aligned} \tag{66}$$

We take $b^N=c^N=\overline{b^N}=\overline{d^N}=0$, and normalize $\langle\Omega|$ and U so that

$$\langle\Omega|=(0\,0\,\cdots\,0\,0) \tag{67}$$

and

$$\sum_\alpha U_{\alpha\beta}=\delta_{N\beta}. \tag{68}$$

U will also diagonalize the exponential in Eq. (39). So we have

$$\mathcal{N}_k(t)=\frac{1}{2\pi i}\sum_{m=-\infty}^{\infty}\oint dz z^{m-k-1}\exp[t\{-B'-\overline{B}'+zC'+z^{-1}\overline{D}'\}]\mathcal{N}'_m(0), \tag{69}$$

where

$$\mathcal{N}'_k(t):=U^{-1}\mathcal{N}_k(t). \tag{70}$$

The matrix in the argument of the exponential in Eq. (69) is diagonal, so the integral can be easily calculated:

$$\mathcal{I}:=\frac{1}{2\pi i}\oint \mathrm{d}z z^{m-k-1}\exp[t(-b^\alpha-\overline{b}^\alpha+zc^\alpha+z^{-1}\overline{d}^\alpha)]. \tag{71}$$

Introducing $w:=\sqrt{(\overline{d}^\alpha/c^\alpha z)}$, one arrives at

$$\mathcal{I}:=\left(\frac{\overline{d}^\alpha}{c^\alpha}\right)^{(m-k)/2}\frac{e^{-t(b^\alpha+\overline{b}^\alpha)}}{2\pi i}\oint dw w^{m-k-1}\exp[\sqrt{c^\alpha\overline{d}^\alpha}t\times(w+w^{-1})], \tag{72}$$

which can be written in terms of modified Bessel functions

$$\mathcal{I}:=\left(\frac{\overline{d}^\alpha}{c^\alpha}\right)^{(m-k)/2}e^{-t(b^\alpha+\overline{b}^\alpha)}I_{k-m}(2\sqrt{c^\alpha\overline{d}^\alpha}t). \tag{73}$$

Then,

$$\mathcal{N}_k(t)=\sum_{m=-\infty}^{\infty}U\,\mathrm{diag}\left\{\left(\frac{\overline{d}^\beta}{c^\beta}\right)^{(m-k)/2}e^{-t(b^\beta+\overline{b}^\beta)}\times I_{k-m}(2\sqrt{c^\beta\overline{d}^\beta}t)\right\}U^{-1}\mathcal{N}_m(0). \tag{74}$$

Note that the right-hand side of Eq. (73) is $\delta_{k,m}$ for $\alpha=N$, since the Nth eigenvalue of B, C, $\overline{B}$, and $\overline{D}$ is zero.

One can start with four special diagonal matrices and then construct the Hamiltonians with different reaction-diffusion rates. Not all diagonal matrices lead to physical stochastic models: negative reaction rates may be obtained. Considering the large-time behavior of average number densities, one can show that

$$|\mathrm{Re}(\sqrt{c^\alpha\overline{d}^\alpha})|\leqslant\mathrm{Re}(b^\alpha+\overline{b}^\alpha), \tag{75}$$

which also shows that

$$\mathrm{Re}(b^\alpha+\overline{b}^\alpha)\geqslant 0. \tag{76}$$

Now, we consider a special choice for U:

$$U^\alpha_\beta=\delta^\alpha_N-(1-\delta^\alpha_N)\delta^\alpha_\beta. \tag{77}$$

Then

$$\begin{aligned}B^\alpha_\beta&=b_\beta(\delta^\alpha_\beta-\delta^\alpha_N),\\ C^\alpha_\beta&=c_\beta(\delta^\alpha_\beta-\delta^\alpha_N),\\ \overline{B}^\alpha_\beta&=\overline{b}_\beta(\delta^\alpha_\beta-\delta^\alpha_N),\\ \overline{D}^\alpha_\beta&=\overline{d}_\beta(\delta^\alpha_\beta-\delta^\alpha_N).\end{aligned} \tag{78}$$

Now, consider

$$\mathcal{A}^{\ \alpha}_{\beta\gamma}=\sum_\lambda H^{\lambda\alpha}_{\beta\gamma}=-b^\alpha\delta^\alpha_\gamma+c^\alpha\delta^\alpha_\beta+(-b_\gamma+c_\beta)\delta^\alpha_N. \tag{79}$$

For $\alpha\neq\gamma$ and $\alpha\neq\beta$,

$$\sum_\lambda H^{\lambda\alpha}_{\beta\gamma}\geqslant 0,\quad \sum_\lambda H^{\lambda\alpha}_{\gamma\beta}\geqslant 0. \tag{80}$$

So, taking $\beta,\gamma\neq N$ and $\alpha=N$,

$$b^\gamma\geqslant c^\beta. \tag{81}$$

The same reasoning is true for $\overline{b}^\gamma$ and $\overline{d}^\beta$:

$$\overline{b}^\gamma\geqslant\overline{d}^\beta. \tag{82}$$

Here, too, as in the previous example, the above choices for B, C, $\overline{B}$, and $\overline{D}$ do not determine H uniquely. One particular solution for the reaction rates is, for $\alpha\neq N$,

$$A_NA_\alpha\rightarrow\begin{cases}A_\alpha A_N, & \Lambda_{N\alpha}\\ A_\alpha A_\alpha, & \overline{d}_\alpha-\Lambda_{N\alpha}\\ A_NA_N, & b_\alpha-\Lambda_{N\alpha},\end{cases} \tag{83}$$

$$A_\alpha A_N\rightarrow\begin{cases}A_NA_\alpha, & \Lambda_{\alpha N}\\ A_\alpha A_\alpha, & c_\alpha-\Lambda_{\alpha N}\\ A_NA_N, & \overline{b}_\alpha-\Lambda_{\alpha N},\end{cases} \tag{84}$$

and, for $\alpha,\beta\neq N$,

$$A_\alpha A_\beta\rightarrow\begin{cases}A_\alpha A_N, & b_\beta-c_\alpha-\Lambda_{\alpha\beta}\\ A_NA_\beta, & \overline{b}_\alpha-\overline{d}_\beta-\Lambda_{\alpha\beta}\\ A_NA_N, & \Lambda_{\alpha\beta}.\end{cases} \tag{85}$$

For $\alpha\neq\beta$, the following reactions may also occur. For $\alpha<\beta$

$$A_\alpha A_\beta\rightarrow\begin{cases}A_\beta A_\alpha, & c_\alpha\\ A_\beta A_\beta, & -c_\alpha+\overline{d}_\beta\end{cases} \tag{86}$$

and for $\alpha>\beta$

$$A_\alpha A_\beta \to \begin{cases} A_\beta A_\alpha, & \overline{d}_\beta \\ A_\alpha A_\alpha, & c_\alpha - \overline{d}_\beta . \end{cases} \tag{87}$$

The constraint of non-negativeness of the reaction rates leads to

$$\begin{aligned} c_\alpha \leqslant d_\beta \leqslant c_\gamma, \quad \alpha < \beta < \gamma, \\ 0 \leqslant \Lambda_{\alpha\beta} \leqslant b_\beta - c_\alpha, \\ \Lambda_{\alpha\beta} \leqslant \overline{b}_\alpha - \overline{d}_\beta, \\ 0 \leqslant \Lambda_{N\alpha} \leqslant \overline{d}_a, \\ 0 \leqslant \Lambda_{N\alpha} \leqslant b_a, \\ 0 \leqslant \Lambda_{\alpha N} \leqslant \overline{b}_a, \\ 0 \leqslant \Lambda_{\alpha N} \leqslant c_a . \end{aligned} \tag{88}$$

4. Type-change invariance

Suppose B, C, $\overline{B}$, and $\overline{D}$ have the property

$$B^{\alpha+\gamma}_{\beta+\gamma} = B^\alpha_\beta, \tag{89}$$

and the same for the other three matrices. Note that the indices of these matrices are defined periodically, so that $N+\alpha$, as an index, is equivalent to α. This is in fact a special case of the commuting matrices discussed earlier. One can use Eq. (74). To do so, one should know the simultaneous eigenvectors of B, C, $\overline{B}$, and $\overline{D}$, and their corresponding eigenvalues. It is not difficult to see that the eigenvectors are

$$U^\alpha_\beta = \frac{1}{\sqrt{N}} \exp\left(\frac{i 2\pi\alpha\beta}{N} \right). \tag{90}$$

The corresponding eigenvectors of B, for example, are

$$b^\beta = \sum_\alpha B^\alpha_0 \exp\left(-\frac{i 2\pi\alpha\beta}{N} \right). \tag{91}$$

Finally, the matrix elements of the inverse of U are

$$(U^{-1})^\alpha_\beta = \frac{1}{\sqrt{N}} \exp\left(-\frac{i 2\pi\alpha\beta}{N} \right). \tag{92}$$

These can be put directly in Eq. (74).

VI. LARGE-TIME BEHAVIOR OF AVERAGE DENSITIES

The large-time behavior of the system is deduced through a steepest-descent analysis of the formal solution (39). One should consider the eigenvalues and the eigenvectors of the z-dependent matrix

$$M(z) := -(B+\overline{B}) + zC + z^{-1}\overline{D}. \tag{93}$$

Denote the eigenvalues of this matrix by $\lambda^\alpha(z)$. As for any value of z, the matrix M has $\langle s|$ as its left eigenvector corresponding to the eigenvalue zero, and it will have a right eigenvector $|w\rangle$ dual to $\langle s|$. $|w\rangle$ is z dependent, but one can normalize it so that

$$\langle s|w(z)\rangle = 1. \tag{94}$$

The fact that $\mathcal{N}$ should not blow up at $t\to\infty$ assures that the real parts of the eigenvalues of $M(z)$ are nonpositive (at least for $|z|=1$). If all the other eigenvalues have negative real parts, then at $t\to\infty$ only $|w\rangle$ survives. That is,

$$\mathcal{N}_k(\infty) = \frac{1}{2\pi i} \sum_m \oint dz z^{m-k-1} |w(z)\rangle\langle s|\mathcal{N}_m(0) = |w(1)\rangle. \tag{95}$$

We have used $\langle s|\mathcal{N}_m(0)=1$. This could also be obtained directly, using the evolution equation (23), by setting $\dot{\mathcal{N}}_k$ equal to zero and assuming $\mathcal{N}_k$ independent of k. So the final state of the system is the eigenvector of $-(B+\overline{B})+C+\overline{D}$, corresponding to the eigenvalue zero.

To investigate the next-to-leading term at $t\to\infty$, consider the other eigenvalues of $M(z)$. Suppose that at $z=z^\alpha_0$ λ^α is stationary. There may be more than one point having this property. So we will have a set consisting of z^α_{0a}'s. Each of these points corresponds to a stationary eigenvalue λ^α_{0a}. We choose that z^α_{0a} for which the corresponding eigenvalue has the largest real part. Denote this point by z_0, its corresponding stationary eigenvalue by λ_0, and its corresponding right eigenvector by $|v_0\rangle$. The next-to-leading term in $\mathcal{N}$ is then

$$\mathcal{N}^{(1)}_k \sim z_0^{-k} e^{t\lambda_0} |v_0\rangle. \tag{96}$$

Note that z_0 is not necessarily a phase; its modulus may be different from 1.

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