Autonomous multispecies reaction-diffusion systems with more-than-two-site interactions

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Abstract

Autonomous multispecies systems with more-than-two-neighbor interactions are studied. Conditions necessary and sufficient for closedness of the evolution equations of the \( n \)-point functions are obtained. The average number of the particles at each site for one species and three-site interactions, and its generalization to the more-than-three-site interactions is explicitly obtained. Generalizations of the Glauber model in different directions, using generalized rates, generalized number of states at each site, and generalized number of interacting sites, are also investigated.

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1 Introduction

The principles of equilibrium statistical mechanics are well established. But, thermal equilibrium is a special case, and little is known about the properties of systems not in equilibrium, for example about the relaxation toward the stationary state. Some interesting problems in non-equilibrium systems are non-equilibrium phase transitions described by phenomenological rate equations, and the way the system relaxes to its steady state. As mean-field techniques, generally, do not give correct results for low-dimensional systems, people are motivated to study exactly-solvable stochastic models in low dimensions. Moreover, solving one-dimensional systems should in principle be easier. Exact results for some models on a one-dimensional lattice have been obtained, for example in [1–12]. 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 [13–27]. Many of the arguments are based on simulation results. There are, however, some exact results as well. For most of the models studied, the interaction is between nearest neighbors.

In [28], a 10-parameter family of stochastic models with interactions between nearest neighbors has been studied. In these models, the $k$-point equal time correlation functions $\langle n_i n_j \cdots n_k \rangle$ satisfy linear differential equations involving no higher-order correlations. We call these models autonomous, in the sense that the evolution equations of $n$-point functions are closed (contain only $n$- or less-point functions). These linear equations for the average number of the particles $\langle n_i \rangle$ have been solved. The same models were studied on lattices with boundaries in [29]. It was shown that these models may exhibit dynamic and static phase transitions. The same idea has been generalized to multi-species models in one dimension with two-site interactions. There, conditions have been obtained that the Hamiltonian should satisfy in order that the evolution equation for correlation functions be closed. The set of equations for average densities can be written in terms of four matrices. 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 the average densities of different species was found. The large-time behaviour of the average densities of different species was also studied. The time evolution equations for more-point functions, generally contain not only these four matrices, but also elements of the Hamiltonian, and to obtain a closed form for their solution is generally not easy.

The Glauber dynamics was originally proposed to study the relaxation of the Ising model near equilibrium states. It was also shown that, there is a relation between the kinetic Ising model at zero temperature and the diffusion annihilation model in one dimension. There is an equivalence between domain walls in the Ising model and particles in the diffusion annihilation model. Kinetic generalizations of the Ising model, for example the Glauber model or the Kawasaki model, are phenomenological models and have been studied extensively [30–41].

In this paper, autonomous multispecies systems with more-than-two-neighbor interactions are studied. Conditions necessary and sufficient for closedness of the evolution equations of the $n$-point functions are obtained. As an example, we obtain explicitly the average number of the particles at each site for one species and three-site interactions. This is then generalized to the case where more than
three site interact. As another example, a generalization of the Glauber model is presented. In this generalization, the processes are the same as those of the ordinary Glauber model, but the rates depend on three free parameters, rather than one free parameter in the ordinary Glauber model. Finally this model is further generalized to the case where the number of interacting sites is more than three and the number of states at each site is more than two.

2 Models leading to closed set of evolution equations

The models addressed are multi-species exclusion reaction-diffusion models. That is, each site is a vacancy or contains one particle. There are several kinds of particles, but at any time at most one kind can be present at each site. Throughout the paper, the system is assumed to be translationally invariant. Consider first a case where the interaction is between three neighboring sites. Then the Hamiltonian describing the system can be written as

\[
\mathcal{H} = \sum_{i=1}^{L} H_{i,i+1,i+2}.
\]  

(1)

The number of sites is $L$ and the number of possible states in a site is $q$ (one of these states, for example the $q$-th one, may be the vacancy); different states of each site are denoted by $\alpha$, $\alpha = 1, \cdots q$. Introducing $n_{i}^{\alpha}$ as the number operator of the particles of type $\alpha$ in the site $i$, we have

\[
\sum_{\alpha=1}^{q} n_{i}^{\alpha} = 1.
\]  

(2)

The average number of the particles of the type $\alpha$ in the site $i$ at the time $t$ is

\[
\langle n_{i}^{\alpha} \rangle = \langle S|n_{i}^{\alpha}|P(t)\rangle,
\]  

(3)

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

\[
\langle S\rangle = \langle s\rangle \otimes \cdots \otimes \langle s\rangle_{L},
\]  

(4)

and

\[
\langle s\rangle := (1 \ 1 \ \cdots 1). \quad (5)
\]  

So, the time evolution of $\langle n_{i}^{\alpha} \rangle$ is given by

\[
\frac{d}{dt} \langle n_{i}^{\alpha} \rangle = \langle S|n_{i}^{\alpha}\mathcal{H}|P(t)\rangle.
\]  

(6)

The only terms of the Hamiltonian $\mathcal{H}$ entering the above equation are $H_{i,i+1,i+2}$, $H_{i-1,i,i+1}$, and, $H_{i-1,i,i+1}$. The result of acting any matrix $Q$ on the bra $\langle s\rangle$ is equal to that of acting the diagonal matrix $\tilde{Q}$ on the same bra, provided
each diagonal element of the matrix \( \tilde{Q} \) is equal to the sum of all elements of the corresponding column in the matrix \( Q \). So, the actions of \((1 \otimes 1 \otimes n^\alpha)H\), \((1 \otimes n^\alpha \otimes 1)H\), and \((n^\alpha \otimes 1 \otimes 1)H\) on \( \langle s \rangle \otimes \langle s \rangle \otimes \langle s \rangle \) are equal to the actions of three diagonal matrices on \( \langle s \rangle \otimes \langle s \rangle \otimes \langle s \rangle \). We use the symbol \( \sim \) to denote the equality of the action on \( \langle s \rangle \otimes \langle s \rangle \otimes \langle s \rangle \). We have

\[
\begin{align*}
(n^\alpha \otimes 1 \otimes 1)H & \sim \sum_{\beta \gamma \lambda} \mathcal{A}^\alpha_{\beta \gamma \lambda} n^\beta \otimes n^\gamma \otimes n^\lambda, \\
(1 \otimes n^\alpha \otimes 1)H & \sim \sum_{\beta \gamma \lambda} \mathcal{A}^\alpha_{\beta \gamma \lambda} n^\beta \otimes n^\gamma \otimes n^\lambda, \\
(1 \otimes 1 \otimes n^\alpha)H & \sim \sum_{\beta \gamma \lambda} \mathcal{A}^\alpha_{\beta \gamma \lambda} n^\beta \otimes n^\gamma \otimes n^\lambda,
\end{align*}
\]

where \( \mathcal{A}^\alpha_{\beta \gamma \lambda} \)'s are defined as

\[
\begin{align*}
1 \mathcal{A}^\alpha_{\beta \gamma \lambda} & := s_\tau s_\omega H^\alpha_{\beta \gamma \lambda}, \\
2 \mathcal{A}^\alpha_{\beta \gamma \lambda} & := s_\sigma s_\omega H^\alpha_{\beta \gamma \lambda}, \\
3 \mathcal{A}^\alpha_{\beta \gamma \lambda} & := s_\tau s_\omega H^\alpha_{\beta \gamma \lambda}.
\end{align*}
\]

An implicit summation (from 1 to \( q \)) over the same subscript and superscript is always assumed. From these, (6) takes the form

\[
\langle \dot{n}^\alpha_i \rangle = \mathcal{A}^\alpha_{\beta \gamma \lambda}(n^\beta_i \gamma_{i+1} \lambda_{i+2}) + 2 \mathcal{A}^\alpha_{\beta \gamma \lambda}(\beta_{i-1} \gamma_i \lambda_{i+1}) + 3 \mathcal{A}^\alpha_{\beta \gamma \lambda}(\beta_{i-2} \gamma_{i-1} \lambda_i) \quad (9)
\]

Generally, the right-hand side of (9) contains one-, two-, and three-point functions. (Note that \( n^\alpha \)'s are not independent.) We want to obtain a condition that only one point functions appear in the right-hand side. To do this, we consider the expression

\[
u = f_{\alpha \beta \gamma} n^\alpha_i n^\beta_j n^\gamma_k,
\]

and ask for the condition that the right-hand side is expressible in terms of linear combinations of \( n^\alpha \)'s, provided

\[
s_\alpha n^\alpha_l = 1.
\]

It is obvious that if

\[
f_{\alpha \beta \gamma} = 1 F_\alpha + 2 F_\beta + 3 F_\gamma,
\]

then the right-hand side of (10) is expressible in terms of linear combinations of \( n^\alpha \)'s. To prove that this form for \( f \) is necessary as well, we just count the number of independent variables in \( f \)'s satisfying the desired property. One can write \( n^\alpha_i \) in terms of one 1 and other \( n^\alpha_l \)'s. Then it is seen that a general cubic form of \( n^\alpha \)'s is expressible in terms of \( q^3 \) independent forms of \( n^\alpha \)'s, each containing no more than three \( n^\alpha \)'s. Of these, \( 1 + 3(q - 1) \) expressions (the monomials of degree zero and one of \( 3(q - 1) \) independent variables) are desirable. The coefficients of other monomials should be zero. So, from \( q^3 \) independent variables in \( f \), there remains only \( 3(q - 1) + 1 \) independent variables in \( f \)'s satisfying the desired
condition. It seems that the right-hand side of (12) contains more independent variables, $3q$. But we note that the transformation

$$iF_\alpha \rightarrow iF_\alpha + _i B,$$  \hspace{1cm} (13)

does not change the right-hand side of (12), provided

$$\sum_i iB = 0.$$  \hspace{1cm} (14)

This means that there are $3 - 1$ redundant variables in the expression (12). So (12) contains actually the correct number of independent variables, and hence is the most general form of $f$ with the desired property.

So, in order that (9) be expressible in terms of only one-point functions, one must have

$$^iA_j^\alpha \rightarrow ^iA_j^\alpha + _j B^\alpha = ^iA_j^\alpha + _j B^\alpha, \hspace{1cm} \text{with} \hspace{1cm} \sum_j _j B^\alpha = 0 \hspace{1cm} (16)$$

does not change the right-hand side of (13).

If (13) is satisfied, (11) takes the form

$$\langle \dot{n}_i^\alpha \rangle = \left( \frac{1}{2} A_j^\alpha + \frac{2}{3} A_j^\alpha + \frac{3}{4} A_j^\alpha \right) \langle n_i^\beta \rangle$$

$$+ \left( \frac{1}{2} A_j^\alpha + \frac{2}{3} A_j^\alpha \right) \langle n_{i+1}^\beta \rangle + \left( \frac{2}{3} A_j^\alpha + \frac{3}{4} A_j^\alpha \right) \langle n_{i-1}^\beta \rangle$$

$$+ \frac{1}{4} A_j^\alpha \langle n_{i+2}^\beta \rangle + \frac{3}{4} A_j^\alpha \langle n_{i-2}^\beta \rangle.$$  \hspace{1cm} (17)

(11) in fact guarantees that the time-evolution equations of $n$-point functions contain only $n$- and less-point functions. In the simplest case, the one-species, each site is vacant or occupied by only one kind of particles. Then, the matrices $^jA$ are two by two.

One can do the same arguments for the case where more than three neighboring sites interact. Suppose the number of interacting sites is $N$. One defines

$$^iA_{\beta_1 \ldots \beta_N}^\alpha := \left( \prod_{l \neq i} s_{\alpha_l} \right) H_{\beta_1 \ldots \beta_N}^{\alpha_1 \ldots \alpha_N}. \hspace{1cm} (18)$$

To ensure that in the time-evolution equation of one-point functions only one-point functions appear, one must have

$$^iA_{\beta_1 \ldots \beta_N}^\alpha = \sum_j ^jA_{\beta_j}^\alpha.$$  \hspace{1cm} (19)

Here too, the gauge transformation (11) does not change the right-hand side of (19), and hence the physics of the problem. It is to be noted that (19) is also sufficient for $n$-point functions evolution equations to contain no more than $n$-point functions.
2.1 Some special cases

We now consider some special cases.

2.1.1 Single species case

In this case the matrices $\mathcal{A}$ are two by two. The time-evolution equation for $\langle n_k \rangle$ will then be

$$\langle \dot{n}_i \rangle = -\alpha \langle n_i \rangle + \beta \langle n_{i+1} \rangle + \beta' \langle n_{i-1} \rangle + \gamma \langle n_{i+2} \rangle + \gamma' \langle n_{i-2} \rangle + \delta. \quad (20)$$

$\delta$ can be eliminated using the redefinition

$$x_i := \langle n_i \rangle - \frac{\delta}{\beta + \beta' + \gamma + \gamma' - \alpha}. \quad (21)$$

Then, introducing the generating function

$$G(z, t) = \sum_{-\infty}^{\infty} x_i z^i, \quad (22)$$

one arrives at,

$$\dot{G}(z, t) = (-\alpha + \beta z^{-1} + \beta' z + \gamma z^{-2} + \gamma' z^2) G(z, t), \quad (23)$$

the solution to which is

$$G(z, t) = \exp \left[ t \left( -\alpha + \beta z^{-1} + \beta' z + \gamma z^{-2} + \gamma' z^2 \right) \right] G(z, 0). \quad (24)$$

Using

$$\exp \left[ \frac{u}{2} \left( z + z^{-1} \right) \right] = \sum_{k=\infty}^{\infty} I_k(u) z^k, \quad (25)$$

one arrives at

$$x_k(t) = e^{-\alpha t} \sum_{j,l=\infty}^{\infty} I_{k-j-2l} \left( 2t \sqrt{\beta' \beta} \right) I_l \left( 2t \sqrt{\gamma' \gamma} \right) \frac{\left( \beta' / \beta \right)^{(k-j-2l)/2} \left( \gamma' / \gamma \right)^{l/2}}{x_j(0)} \cdot \quad (26)$$

A similar procedure can be done for more-than-three-neighboring-site interactions. The main difference will be the number of modified Bessel functions appearing in the expression.

2.1.2 Generalizations of the Glauber model

Consider a two-state three-neighbor interaction of the form

$$\mathcal{A}_{\beta \gamma \lambda} = 0, \quad (27)$$

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This means that, similar to the Glauber model, any site interacts only with its neighboring sites. The interactions are

\[
\begin{align*}
AAA &\rightarrow A\emptyset A & \mu_1 \\
\emptyset\emptyset\emptyset &\rightarrow \emptyset A\emptyset & \mu_2 \\
A\emptyset A &\rightarrow AA A & \lambda_1 \\
\emptyset A\emptyset &\rightarrow \emptyset\emptyset\emptyset & \lambda_2 \\
AA\emptyset &\rightarrow A\emptyset\emptyset & \alpha_1 \\
\emptyset\emptyset A &\rightarrow \emptyset A A & \alpha_2 \\
A\emptyset\emptyset &\rightarrow AA\emptyset & \beta_1 \\
\emptyset A A &\rightarrow \emptyset\emptyset A & \beta_2.
\end{align*}
\]

This is a generalization of the Glauber model. For the ordinary Glauber model

\[
\begin{align*}
\mu_1 &= \mu_2 = 1 - \tanh \frac{J}{k_B T} \\
\lambda_1 &= \lambda_2 = 1 + \tanh \frac{J}{k_B T} \\
\alpha_1 &= \alpha_2 = \beta_1 = \beta_2 = 1
\end{align*}
\]

The criterion \cite{19} for the closedness of the evolution-equation for one-point functions results in the following relations between the rates in the generalized Glauber model.

\[
\begin{align*}
\mu_i - \alpha_i &= \beta_j - \lambda_j \quad \text{for any } i, j \\
\alpha_1 + \beta_1 &= \alpha_2 + \beta_2
\end{align*}
\]

So there are four independent variables in terms of them the above eight parameters can be expressed. One can write the expressions as

\[
\begin{align*}
\mu_1 &= A - B - C - C' \\
\mu_2 &= A + B \\
\lambda_1 &= A + B + C + C' \\
\lambda_2 &= A - B \\
\alpha_1 &= A - B - C' \\
\alpha_2 &= A + B + C \\
\beta_1 &= A + B + C' \\
\beta_2 &= A - B - C.
\end{align*}
\]

Of course one of the parameters can be absorbed through a time-rescaling. The resulting evolution-equation for the average particle-number is

\[
\langle \dot{n}_i \rangle = A + B - 2A\langle n_i \rangle + C\langle n_{i+1} \rangle + C'\langle n_{i-1} \rangle,
\]

which is easy to solve.

This generalized Glauber model can further be generalized in two directions: when the number of the interacting sites is more than 3, and when the number of states of each site is more than 2. The first case means that the interaction
is in a block of length $N$, resulting in the change of the state of a single specific site in that block. This rate of change depends on the states of this site and the states of the other $N - 1$ sites. Let’s label this specific site of the block by $0$. (Usually the length of the block is considered to be an odd integer ($2k + 1$), and the evolving site is assumed to be the central one.) Denote the state of the site $i$ by $\sigma_i$, where $\sigma_i$ can take the values 1 (particle) or 0 (vacancy). Then the evolution equation for the average particle number is

$$\langle \dot{n}_0 \rangle = -\left\langle \sum_{\sigma} R(1, \sigma) n_0 \prod_{i \neq 0} \left[ 1 - n_i + \sigma_i(2n_i - 1) \right] \right\rangle$$

$$+ \left\langle \sum_{\sigma} R(0, \sigma)(1 - n_0) \prod_{i \neq 0} \left[ 1 - n_i + \sigma_i(2n_i - 1) \right] \right\rangle. \quad (33)$$

Here the state of other interacting sites is denoted by $\vec{\sigma}$, $R(\sigma_0, \vec{\sigma})$ is the rate of change of the state of site 0, from $\sigma_0$ to $1 - \sigma_0$, when the states of the other interacting sites is $\vec{\sigma}$.

We are looking for those rates $R(\sigma_0, \vec{\sigma})$ that make the right-hand side of this evolution equation a linear combination of $\langle n_i \rangle$’s. The claim is that the general form of these rates is

$$R(\sigma_0, \vec{\sigma}) = A + (-1)^{\sigma_0} \left( B + \sum_{i \neq 0} C_i \sigma_i \right). \quad (34)$$

Inserting this ansatz into the evolution equation (33) we get

$$\langle \dot{n}_0 \rangle = B + A(1 - 2n_0) + \sum_{i \neq 0} C_i \langle n_i \rangle. \quad (35)$$

So it is clear that the ansatz (34) leads into a closed set of evolution-equations for the average particle number. It remains to prove that this ansatz is the most general one satisfying this property. To see this, one considers (33). In the right-hand side of this equation there are $2^N$ terms (the expectation of monomials in terms of $n_i$’s). Of these, we wish that the coefficients of all be zero, except for the coefficients of the constant term, and linear terms. So, there are $2^N - (N + 1)$ equations to be satisfied for the rates (consisting themselves of $2^N$ unknowns). This shows that the rates satisfying the desired property contain $N + 1$ independent variables, and it is clear that the ansatz (34) contains $N + 1$ independent variables. So it is the most general solution.

Now consider the second generalization, when the number of possible states at each site is more than 2, say $q$, and each block consists of $N$ sites. The state of the site $i$ is denoted by $\sigma_i$, which can take $q$ values. That site the state of which is denoted by 0. The rate of change of the state of the site 0 from $\beta$ to $\alpha$ is denoted by $R^\beta_{\beta, \sigma}$. The evolution equation for the average numbers is then

$$\langle \dot{n}_0^\alpha \rangle = \left\langle \sum_{\sigma} \sum_{\beta \neq \alpha} R^\alpha_{\beta, \sigma} n_0^\beta \prod_{i \neq 0} n_i^{\sigma_i} \right\rangle$$

$$- \left\langle \sum_{\sigma} \sum_{\beta \neq \alpha} R^\beta_{\alpha, \sigma} n_0^\alpha \prod_{i \neq 0} n_i^{\sigma_i} \right\rangle. \quad (36)$$
Defining

\[ R_{\alpha,\vec{\sigma}}^\alpha := - \sum_{\beta \neq \alpha} R_{\alpha,\vec{\sigma}}^\beta, \]  

(37)

the evolution equation reads

\[ \langle \dot{\eta}_0^\alpha \rangle = \sum_{\vec{\sigma}} R_{\beta,\vec{\sigma}}^\alpha \left( n_0^\beta \prod_{i \neq 0} n_i^{\sigma_i} \right). \]  

(38)

It is easy to see that for the right-hand side of this equation be expressible in terms of one-point functions, one should have

\[ R_{\beta,\vec{\sigma}}^\alpha = 0 R_{\beta}^\alpha + \sum_{i \neq 0} R_{\sigma_i}^\alpha, \]  

(39)

Note that this is nothing but

\[ 0 A_{\beta,\vec{\sigma}}^\alpha = \sum_i 0 A_{\sigma_i}^\alpha, \]  

(40)

obtained in (19). In this case, other \(^0 A\)'s vanish. The evolution equation of the one-point functions is then

\[ \langle \dot{\eta}_0^\alpha \rangle = \sum_i R_{\beta}^\alpha \langle n_i^\beta \rangle. \]  

(41)

Previous discussions shows that this is the most general form of the rates for them the evolution-equations of the one-point functions contain only one-point functions. Here too, there is a gauge freedom in choosing \(^i R\)'s, namely

\[ i R_{\beta}^\alpha \rightarrow i R_{\beta}^\alpha + i B^\alpha s_{\beta}, \quad \text{with} \quad \sum_i i B^\alpha = 0. \]  

(42)

This is the same gauge freedom encountered with earlier, (16).
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