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p-species integrable reaction–diffusion processes

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Abstract

We consider a process in which there are p-species of particles, i.e. $A_1, A_2, \ldots, A_p$, on an infinite one-dimensional lattice. Each particle A_i can diffuse to its right neighbouring site with rate D_i, if this site is not already occupied. Also they have the exchange interaction $A_j + A_i \rightarrow A_i + A_j$ with rate r_{ij}. We study the range of parameters (interactions) for which the model is integrable. The wavefunctions of this multi-parameter family of integrable models are found. We also extend the two-species model to the case in which the particles are able to diffuse to their right or left neighbouring sites.

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1. Introduction

Our understanding of nonequilibrium statistical physics is far behind that for the equilibrium theory. Even simple models may pose a formidable problem if one wants to approach them analytically. As interesting example of stochastic models, which may be investigated analytically in a few cases, is one-dimensional reaction–diffusion processes which are of both theoretical and experimental interest in a very wide context of physics and chemistry, such as stochastic spin-flip dynamics [1], traffic flow [2, 3], the kinetics of bipolymerization [4, 5], reptation of DNA in gels [6, 7], interface growth [8, 9], diffusion in zeolites [10, 11] and many other phenomena.

Asymmetric simple exclusion processes (ASEP) in one dimension is one of the simplest examples of a driven diffusion system [12, 13]. For example, the totally ASEP model describes a process in which each lattice site can be occupied by at most one particle and the particles hop to their right neighbouring sites if they are not already occupied, with a rate which is the same for all particles, otherwise the attempted move is rejected. The dynamics of these models can be fully specified by a master equation and an appropriate boundary condition, which imposed

on the probabilities appear in the master equation. Using the coordinate Bethe ansatz, the author of [14] has exactly obtained the N-particle conditional probabilities of totally ASEP, in which the particles can move to the left and right with different rates.

Now the interesting point is that if one changes the boundary condition, without altering the master equation, one can model another reaction–diffusion processes even with long-range interactions. For example, in [15], the so-called generalized totally ASEP model has been exactly solved in this way. In this model the particle hops to the next right site by pushing all the neighbouring particles to their next right sites, with a rate depending on the number of right neighbouring particles. The partially generalized ASEP model has also been studied in [16]. Note that in all these cases, the solvability of the models is shown by proving the factorization of N-particle S-matrices into two-particle ones, which were found exactly.

In all the above ASEPs, there is only one species of particle, that is all the particles are of the same type. But if one considers problems involving two or more species, the situation becomes more complicated. The main complexity arises from the fact that the above mentioned factorization of N-particle systems reduces to the condition of satisfying the two-particle S-matrices in the quantum Yang–Baxter equation (QYBE). In one-species models, the S-matrices are not really matrices, they are c-numbers and therefore their satisfying the QYBE becomes trivial. This new condition can hardly restrict the number of solvable models with more than one species particles. In [17], a class of two species reaction–diffusion processes with the following properties has been considered: (1) the particles diffuse to their right neighbouring sites, (2) they can be annihilated or created, but the total number of particles is constant and (3) the interaction rates are all the same. It is shown that among 4096 types of models with the above properties, which can be modelled by a master equation and a number of boundary conditions, there are only 28 independent interactions whose two-particle S-matrices satisfy the QYBE and therefore are solvable. The third condition (equality of the interaction rates) was very crucial in the proof of solvability.

In this paper we want to study the effect of interaction rates in solvability of p-species reaction–diffusion processes, by considering a specific model. We begin our investigation by choosing one of the two-species interactions that has been introduced in [17], but with different interaction rates, and try to obtain the range of parameters to ensure the solvability of the corresponding extended p-species model. As we show, we must restrict ourselves to a narrower and narrower range of parameters, as we go ahead, and finally arrive at a model with a specific relation between the interaction rates and also a specific range for these rates.

The plan of the paper is as follows. In section 2, we begin with the following two-species reaction–diffusion processes:

$$A + \emptyset \xrightarrow{D_A} \emptyset + A \qquad B + \emptyset \xrightarrow{D_B} \emptyset + B \qquad A + B \xrightarrow{s} B + A \qquad B + A \xrightarrow{r} A + B \tag{1}$$

and write down a master equation and a number of boundary conditions to describe the dynamics of these interactions. D_A and D_B are the right-diffusion rates of A and B particles, respectively, and s and r are the rates of transforming (exchanging) A and B particles with each other for $(\ldots AB\ldots)$ and $(\ldots BA\ldots)$ configurations, respectively. We will show that only for the $D_A = D_B = 1$ case does there exist the coordinate Bethe ansatz solution for probabilities (note that taking $D \equiv 1$ is in fact a choosing of time scale). Moreover, we will see that the consistency of the solutions (which will appear as satisfying the two-particle S-matrix in QYBE) restricts us to $r = 0$ or $s = 0$ cases (which are the same after relabelling $A \leftrightarrow B$). We therefore conclude that the solvable model (interaction) is the following one-parameter

family process:

$$A+\emptyset \xrightarrow{1} \emptyset + A \qquad B+\emptyset \xrightarrow{1} \emptyset + B \qquad B + A \xrightarrow{r} A + B. \tag{2}$$

Note that for $r = 1$, interactions (2) are one of the 28 interactions introduced in [17]. We then generalize the interactions (2) to a p-species model in which the particles A_i $(i = 1, \ldots, p)$ can diffuse to their right neighbouring sites, all with equal rate 1, and also have exchange interactions with different rates:

$$A_i + \emptyset \xrightarrow{1} \emptyset + A_i \qquad A_j + A_i \xrightarrow{r_{ij}} A_i + A_j \qquad (j > i). \tag{3}$$

We label the species such that the configuration $(\ldots A_j A_i \ldots)$ can go to $(\ldots A_i A_j \ldots)$, only when $j > i$, therefore r in equation (2) is in fact r_{12}. After a lengthy calculation, we show that there must be a specific relation between r_{ij}s until the $p^2 \times p^2$ two-particle S-matrix satisfies the QYBE.

In section 3, we calculate the two-particle conditional probabilities of reaction (2), and show that only for $0 \leqslant r < 2$ are we able to calculate these probabilities by a standard superposition of the eigenfunctions with real eigenvalues. The long-time behaviour of the probabilities is also discussed. Finally, in section 4, we generalize the reactions (2) to the case where the particles can diffuse towards both right and left:

$$\begin{aligned} &A+\emptyset \xrightarrow{D_R} \emptyset + A \qquad B+\emptyset \xrightarrow{D_R} \emptyset + B \qquad \emptyset + A \xrightarrow{D_L} A + \emptyset \\ &\emptyset + B \xrightarrow{D_L} B + \emptyset \qquad B + A \xrightarrow{r} A + B \qquad A + B \xrightarrow{s} B + A. \end{aligned} \tag{4}$$

We show that there must be a fine tuning of parameters if one demands the reactions (4) to be solvable.

2. p-species exchange–diffusion processes

2.1. The master equation for the two-species case

Consider the interactions introduced in equation (1). The basic quantities that must be calculated are the probabilities $P_{\alpha_1\alpha_2\cdots\alpha_N}(x_1, x_2, \ldots, x_N; t)$ for finding at time t the particle of type α_1 at site x_1, particle of type α_2 at site x_2, etc. Each α_i can be A or B. Following [14], we take these functions to define probabilities only in the physical region $x_1 < x_2 < \cdots < x_N$, and the regions where any two adjacent coordinates are equal are the boundaries of the physical region. For $x_{i-1} - x_i > 1\ \forall i$, the particles can only hop to their right neighbouring sites and therefore the master equation is

$$\begin{aligned} \frac{\partial}{\partial t} P_{\alpha_1\alpha_2\cdots\alpha_N}(x_1, x_2, \ldots, x_N; t) = \sum_{i=1}^{N} D_{\alpha_i} [&P_{\alpha_1\alpha_2\cdots\alpha_N}(x_1, \ldots, x_{i-1}, x_i - 1, x_{i+1}, \ldots, x_N; t) \\ &- P_{\alpha_1\alpha_2\cdots\alpha_N}(x_1, x_2, \ldots, x_N; t)] \end{aligned} \tag{5}$$

where the first N terms are the sources of $P_{\alpha_1\alpha_2\cdots\alpha_N}(x_1, x_2, \ldots, x_N; t)$ and the second N terms are the sinks of it. It is obvious that if $x_{i+1} = x_i + 1$ for some i's, then some of the probability functions on the right-hand side of equation (5) go out from the physical region. So we need to specify the boundary terms. The specification of these terms depends on the details of the interactions of the particles. For exchange interactions defined in equation (1), the suitable boundary conditions are:

$$\begin{aligned} &D_A P_{BA}(x, x) = s P_{AB}(x, x+1) + (D_B - r) P_{BA}(x, x+1) \\ &D_B P_{AB}(x, x) = r P_{BA}(x, x+1) + (D_A - s) P_{AB}(x, x+1) \\ &P_{\alpha\alpha}(x, x) = P_{\alpha\alpha}(x, x+1) \qquad (\alpha = A, B) \end{aligned} \tag{6}$$

in which the time variable and all the other coordinates have been suppressed for simplicity. To justify these boundary conditions, it is enough to examine them in some specific cases. Let us do it for a rather complicated case, for example $P_{ABBA}(x, x+1, x+2, x+3)$. From master equation (5), we have

$$\frac{\partial}{\partial t}P_{ABBA}(x,x+1,x+2,x+3) = D_A P_{ABBA}(x-1,x+1,x+2,x+3) + D_B P_{ABBA}(x,x, x+2,x+3) + D_B P_{ABBA}(x,x+1,x+1,x+3) + D_A P_{ABBA}(x,x+1, x+2,x+2) - 2(D_A+D_B)P_{ABBA}(x,x+1,x+2,x+3). \tag{7}$$

If we use the relations (6) in the second, third and fourth terms on the right-hand side of (7), we find

$$\frac{\partial}{\partial t}P_{ABBA}(x,x+1,x+2,x+3) = D_A P_{ABBA}(x-1,x+1,x+2,x+3) + r P_{BABA}(x,x+1,x+2,x+3) + s P_{ABAB}(x,x+1,x+2,x+3) - (D_A+r+s)P_{ABBA}(x,x+1,x+2,x+3). \tag{8}$$

This equation is exactly what we expect from interactions (1), because the source terms of configuration $(\ldots\emptyset ABBA\emptyset\ldots)$ are: $(\ldots A\emptyset BBA\emptyset\ldots)$ (with rate D_A), $(\ldots\emptyset BABA\emptyset\ldots)$ (with rate r) and $(\ldots\emptyset ABAB\emptyset\ldots)$ (with rate s), and its sink terms: $(\ldots\emptyset ABB\emptyset A\ldots)$ (with rate D_A), $(\ldots\emptyset BABA\emptyset\ldots)$ (with rate s) and $(\ldots\emptyset ABAB\emptyset\ldots)$ (with rate r). It can be shown that the boundary conditions (6) results in the correct terms for any desired configuration.

2.2. The Bethe ansatz solution (two-species)

Now we want to solve the master equation (5) with boundary conditions (6) by the coordinate Bethe ansatz method. First we define $\Psi_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N)$ through

$$P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N;t) = \mathrm{e}^{-\epsilon_N t}\Psi_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N) \tag{9}$$

and then substitute it in equation (5), which results in

$$\sum_{i=1}^{N} D_{\alpha_i}\Psi_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_{i-1},x_i-1,x_{i+1},\ldots,x_N) = \left(\sum_{i=1}^{N} D_{\alpha_i} - \epsilon_N\right)\Psi_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N). \tag{10}$$

To solve this equation, we use the coordinate Bethe ansatz for each of the components $\Psi_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N)$:

$$\Psi_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N) = \sum_{\sigma} A_{\sigma}^{(\alpha_1\cdots\alpha_N)}\,\mathrm{e}^{\mathrm{i}\sigma(\boldsymbol{p})\cdot\boldsymbol{x}} \tag{11}$$

where $\boldsymbol{x}$ and $\boldsymbol{p}$ stand for N-tuple coordinates and momenta, respectively, and $\sigma(\boldsymbol{p})$ is a permutation of momenta. The sum is over all permutations. Inserting (11) into (10) yields

$$\sum_{\sigma}\left[\epsilon_N - \sum_{j=1}^{N} D_{\alpha_j} + \sum_{j=1}^{N} D_{\alpha_j}\mathrm{e}^{-\mathrm{i}\sigma(p_j)}\right] A_{\sigma}^{(\alpha_1\cdots\alpha_N)}\,\mathrm{e}^{\mathrm{i}\sigma(\boldsymbol{p})\cdot\boldsymbol{x}} = 0. \tag{12}$$

As $A_{\sigma}^{(\alpha_1\cdots\alpha_N)}\,\mathrm{e}^{\mathrm{i}\sigma(\boldsymbol{p})\cdot\boldsymbol{x}}$ are linearly independent for different σ, the only solution of equation (12) is

$$\epsilon_N - \sum_{j=1}^{N} D_{\alpha_j} + \sum_{j=1}^{N} D_{\alpha_j}\,\mathrm{e}^{-\mathrm{i}\sigma(p_j)} = 0 \qquad \forall\sigma \tag{13}$$

or

$$\sum_{j=1}^{N} D_{\alpha_j} \mathrm{e}^{-\mathrm{i}\sigma_1(p_j)} = \sum_{j=1}^{N} D_{\alpha_j} \mathrm{e}^{-\mathrm{i}\sigma_2(p_j)} = \cdots = \sum_{j=1}^{N} D_{\alpha_j} \mathrm{e}^{-\mathrm{i}\sigma_n(p_j)} \tag{14}$$

where n is the number of elements of the permutation group. As these equalities must hold for an arbitrary $\boldsymbol{p}$, the only nontrivial solution is

$$D_A = D_B \equiv 1. \tag{15}$$

Now as for any group element σ we have

$$\sum_{j=1}^{N} \mathrm{e}^{-\mathrm{i}\sigma(p_j)} = \mathrm{e}^{-\mathrm{i}p_1} + \cdots + \mathrm{e}^{-\mathrm{i}p_N} \tag{16}$$

the equalities (14) are satisfied satisfactorily. Therefore, the Bethe ansatz solution exists only for equal diffusion rates, in which case the eigenvalue ϵ_N is found to be (by equation (13)):

$$\epsilon_N = \sum_{j=1}^{N} (1 - \mathrm{e}^{-\mathrm{i}p_j}). \tag{17}$$

It is easier to consider $\Psi_{\alpha_1 \cdots \alpha_N}(x_1, \ldots, x_N)$ and $A_\sigma^{(\alpha_1 \cdots \alpha_N)}$ as the components of the tensors $\boldsymbol{\Psi}$ and $\mathbf{A}_\sigma$ with rank N, respectively. Therefore equation (11) can be written as

$$\boldsymbol{\Psi}(x_1, \ldots, x_N) = \sum_{\sigma} \mathbf{A}_\sigma \, \mathrm{e}^{\mathrm{i}\sigma(\boldsymbol{p})\cdot\boldsymbol{x}}. \tag{18}$$

The boundary conditions of $\boldsymbol{\Psi}$ can be obtained by substituting equation (9) in (6), with $D_A = D_B \equiv 1$. The resulting equation is

$$\boldsymbol{\Psi}(\ldots, \zeta, \zeta, \ldots) = \mathbf{b}_{k,k+1} \boldsymbol{\Psi}(\ldots, \zeta, \zeta + 1, \ldots) \tag{19}$$

where

$$\mathbf{b}_{k,k+1} = \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes \underbrace{\mathbf{b}}_{k,k+1} \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \tag{20}$$

with

$$\mathbf{b} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1-s & r & 0 \\ 0 & s & 1-r & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{21}$$

The coefficients $\mathbf{A}_\sigma$ in equation (18) must be found by substituting the wavefunction (18) into the boundary condition (19), which yields

$$\sum_{\sigma} \mathrm{e}^{\mathrm{i} \sum_{j \neq k,k+1} \sigma(p_j) x_j + \mathrm{i}(\sigma(p_k) + \sigma(p_{k+1}))\xi} (1 - \mathrm{e}^{\mathrm{i}\sigma(p_{k+1})} \mathbf{b}_{k,k+1}) \mathbf{A}_\sigma = 0. \tag{22}$$

As the exponential part of equation (22) is symmetric with respect to $p_k \leftrightarrow p_{k+1}$, if we also symmetrize the remaining terms with respect to this interchange, we obtain

$$(1 - \mathrm{e}^{\mathrm{i}\sigma(p_{k+1})} \mathbf{b}_{k,k+1}) \mathbf{A}_\sigma + (1 - \mathrm{e}^{\mathrm{i}\sigma(p_k)} \mathbf{b}_{k,k+1}) \mathbf{A}_{\sigma\sigma_k} = 0 \tag{23}$$

where σ_k represents the permutation group element which only interchanges p_k and p_{k+1}.

Therefore

$$\mathbf{A}_{\sigma\sigma_k} = \mathbf{S}_{k,k+1}(\sigma(p_k), \sigma(p_{k+1}))\mathbf{A}_\sigma \tag{24}$$

where

$$\mathbf{S}_{k,k+1}(z_1, z_2) = \mathbf{1}\otimes\cdots\otimes\mathbf{1}\otimes\underbrace{S(z_1, z_2)}_{k,k+1}\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1} \tag{25}$$

in which

$$\mathbf{S}(z_1, z_2) = -(\mathbf{1} - z_1\mathbf{b})^{-1}(\mathbf{1} - z_2\mathbf{b}). \tag{26}$$

In the above equations, z_k stands for $\mathrm{e}^{\mathrm{i}p_k}$. In this way, all the $\mathbf{A}_\sigma$ coefficients are determined in terms of $\mathbf{A}_1$ which is fixed by the initial conditions (the particles' positions at $t = 0$). It seems that we have solved the problem for arbitrary $\mathbf{b}$ (i.e. interaction), but it is not true (note that we have not yet used the explicit form of $\mathbf{b}$ in deriving $\mathbf{A}_\sigma$). The crucial point is that $\sigma_1\sigma_2\sigma_1$ and $\sigma_2\sigma_1\sigma_2$ are equal as elements of the permutation group, therefore we should impose the following condition on the corresponding $\mathbf{A}_\sigma$

$$\mathbf{A}_{\sigma_1\sigma_2\sigma_1} = \mathbf{A}_{\sigma_2\sigma_1\sigma_2} \tag{27}$$

and this highly restricts the allowed $\mathbf{b}$ matrices (i.e. interactions). It can be shown that equation (27) reduces to the following relation for $S(z_1, z_2)$ matrices (see [17] for more details):

$$(S(w,t)\otimes 1)(1\otimes S(z,t))(S(z,w)\otimes 1) = (1\otimes S(z,w))(S(z,t)\otimes 1)(1\otimes S(w,t)) \tag{28}$$

in which $z = \mathrm{e}^{\mathrm{i}p_1}$, $w = \mathrm{e}^{\mathrm{i}p_2}$, and $t = \mathrm{e}^{\mathrm{i}p_3}$. Note that equation (28) is nothing but the quantum Yang–Baxter equation.

Now if one calculates the S-matrix from equation (26), using $\mathbf{b}$ from (21), the QYBE (28) reduces to an 8×8 matrix with 14 nonzero elements (after writing equation (28) as RHS – LHS $= 0$) that must be equated to the zero matrix. The elements are functions of p_1, p_2, p_3, r and s which all must be equal to zero for arbitrary momentum values p_1, p_2 and p_3. It can be shown that the unique solutions of these 14 equations are:

$$\begin{array}{lll} \text{solution 1:} & r = 0 & \text{arbitrary } s \\ \text{solution 2:} & s = 0 & \text{arbitrary } r. \end{array} \tag{29}$$

As these two solutions are equivalent (by relabelling $A \leftrightarrow B$), so the only integrable model is the one indicated in equation (2).

2.3. The p-species model

Now let us generalize the reaction (2) to the case where there exist p kinds of particles, which we label by $A_1, A_2, \ldots, A_p$. Each particle can diffuse to its right neighbouring site, and any two particles can exchange with each other. From the results obtained in the previous subsection, we know that if we want the model to be integrable, we must restrict ourselves to the case where the particles' diffusion rates are equal (scaled to one), and also for each of the two particles there is only one allowed exchange interaction. For example $A_2 + A_1 \to A_1 + A_2$ is allowed, but $A_1 + A_2 \to A_2 + A_1$ is forbidden. We label the particles such that $A_j + A_i \to A_i + A_j$ is allowed only for $j > i$, and denote the reaction rate of this interaction by r_{ij}, see equation (3).

The master equation of this p-species model is again equation (5) (with $D_{\alpha_i} = 1$), but now each α_i can be $A_1, A_2, \ldots, A_p$. The boundary conditions are the generalization of equation (6) but now for each two-particle species A_i and A_j, i.e. $P_{AB} \to P_{ij}$, $P_{BA} \to P_{ji}$, $s = 0$, $D_A = D_B = 1$, and $r \to r_{ij}$; so

$$\begin{aligned} P_{ij}(x,x) &= P_{ij}(x,x+1) + r_{ij}P_{ji}(x,x+1) \qquad j > i \\ P_{ji}(x,x) &= (1-r_{ij})P_{ji}(x,x+1) \qquad j > i \\ P_{ii}(x,x) &= P_{ii}(x,x+1). \end{aligned} \tag{30}$$

The wavefunctions can again be factorized by equation (9), and the coordinate Bethe ansatz solution (18) is still valid. The boundary conditions can be rewritten as (19), but here $\mathbf{b}$ is the following $p^2 \times p^2$ matrix:

$$\mathbf{b} = \sum_{i \leqslant j} E_{ii} \otimes E_{jj} + \sum_{i<j} r_{ij} E_{ij} \otimes E_{ji} + \sum_{i>j} (1 - r_{ji}) E_{ii} \otimes E_{jj} \tag{31}$$

where E_{ij} is a $p \times p$ matrix with elements $(E_{ij})_{kl} = \delta_{ik}\delta_{jl}$. It can be shown that the S-matrix (26) becomes

$$S(z,w) = \sum_{i,j=1}^{p} \frac{1 - w(1 - r'_{ji})}{(1 - r'_{ji})z - 1} E_{ii} \otimes E_{jj} + \sum_{i,j=1}^{p} r'_{ij} \frac{z - w}{(z-1)(1 - z + z r'_{ij})} E_{ij} \otimes E_{ji} \tag{32}$$

in which

$$r'_{ij} = \begin{cases} 0 & \text{if } i \geqslant j \\ r_{ij} & \text{if } i < j. \end{cases} \tag{33}$$

Now expression (32) must satisfy the QYBE (28). After a lengthy calculation, it can be shown that the only nontrivial solutions of QYBE are the following (for each $i < j < k$ indices):

$$\begin{array}{lll} \text{solution 1:} & r_{ij} = 0 & r_{ik} \text{ and } r_{jk} \text{ arbitrary} \\ \text{solution 2:} & r_{ik} = 0 & r_{jk} = 0 \text{ and } r_{ij} \text{ arbitrary} \\ \text{solution 3:} & r_{ij} = r_{ik} & r_{jk} \text{ arbitrary.} \end{array} \tag{34}$$

For any set of interaction rates where each three of them satisfies any of the solutions 1, 2 or 3, with the constraint that the relations between r_{ij} must be consistent in all subsets, we have an integrable p-species model with wavefunction (18) whose coefficients are determined by equation (24) and the S-matrix introduced in (32).

For $p = 3$, the allowed sets of interaction rates are exactly the same as the three solutions (34) with $(ijk) = (123)$. But for $p > 3$ cases, we can choose different consistent solutions for any (ijk) and therefore extracting all the allowed sets is not so easy. For example, for $p = 4$, in which there are six interaction rates $r_{12}, r_{13}, r_{14}, r_{23}, r_{24}$, and r_{34}, the allowed sets

of parameters are as follows:

$$\begin{aligned}
&\{r_{14}, r_{24}, r_{34}\}\\
&\{r_{12}, r_{34}\}\\
&\{r_{13}, r_{23}\}\\
&\{r_{13}, r_{24}\}\\
&\{r_{14}, r_{23}\}\\
&\{r_{14}, r_{34}, r_{23} = r_{24}\}\\
&\{r_{24}, r_{34}, r_{12} = r_{14}\}\\
&\{r_{24}, r_{34}, r_{13} = r_{14}\}\\
&\{r_{24}, r_{34}, r_{12} = r_{13} = r_{14}\}\\
&\{r_{13}, r_{23} = r_{24}\}\\
&\{r_{23}, r_{12} = r_{13}\}\\
&\{r_{23}, r_{13} = r_{14}\}\\
&\{r_{23}, r_{12} = r_{13} = r_{14}\}\\
&\{r_{34}, r_{13} = r_{14}, r_{23} = r_{24}\}\\
&\{r_{34}, r_{12} = r_{13} = r_{14}, r_{23} = r_{24}\}.
\end{aligned} \tag{35}$$

Note that in all the above allowed sets, we have only shown the free parameters and the relations that must be satisfied by them, and the zero reaction rates have not been written. In this way we find a large class of multi-parameter p-species integrable reaction–diffusion models.

3. Two-particle conditional probabilities for a two-species model

Now for the simplest case, that is the two-species reactions (2), let us calculate the two-particle conditional probabilities $P(\alpha_1, \alpha_2, x_1, x_2; t|\beta_1, \beta_2, y_1, y_2; 0)$, which is the probability of finding particles α_1 and α_2 at time t at sites x_1 and x_2, respectively, if at $t = 0$ we have the particles β_1 and β_2 at sites y_1 and y_2, respectively. These probabilities can be found by a linear combination of eigenfunctions $P(x_1, x_2)$. Therefore,

$$\begin{pmatrix} P_{AA}\\ P_{AB}\\ P_{BA}\\ P_{BB}\end{pmatrix}(\boldsymbol{x}; t|\beta, \boldsymbol{y}; 0) = \int f(p_1, p_2)\mathrm{e}^{-\epsilon_2 t}\boldsymbol{\Psi}(x_1, x_2)\,\mathrm{d}p_1\,\mathrm{d}p_2$$

$$= \frac{1}{(2\pi)^2}\int \mathrm{e}^{-\epsilon_2 t}\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{y}}\left\{\begin{pmatrix} a\\ b\\ c\\ d\end{pmatrix}\mathrm{e}^{\mathrm{i}(p_1x_1+p_2x_2)} + S_{12}(p_1, p_2)\begin{pmatrix} a\\ b\\ c\\ d\end{pmatrix}\mathrm{e}^{\mathrm{i}(p_2x_1+p_1x_2)}\right\}\mathrm{d}p_1\,\mathrm{d}p_2. \tag{36}$$

In this expansion, $P(\boldsymbol{x}; t|\beta, \boldsymbol{y}; 0)$ stands for $P(\alpha_1, \alpha_2, x_1, x_2; t|\beta_1, \beta_2, y_1, y_2; 0)$ and $f(p_1, p_2)$ is the coefficient of expansion, where in the second equality we choose it to be $\frac{1}{(2\pi)^2}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{y}}$ (see [14–17]). $\epsilon_2 = 2 - \mathrm{e}^{-\mathrm{i}p_1} - \mathrm{e}^{-\mathrm{i}p_2}$ (see (17)) and $\boldsymbol{\Psi}$ is the two-particle wavefunction (18), in which equation (24) has been used for $\mathbf{A}_{\sigma_1}$ ($\mathbf{A}_{\sigma_1} = S_{12}(p_1, p_2)\mathbf{A}_1$). The column matrix

$$\begin{pmatrix} a\\ b\\ c\\ d\end{pmatrix}$$

stands for $\mathbf{A}_1$, whose components must be determined by initial conditions, and $S_{12}(p_1, p_2)$ is

$$S_{12}(p_1, p_2) = \begin{pmatrix} s_1 & 0 & 0 & 0 \\ 0 & s_1 & s_2 & 0 \\ 0 & 0 & s_3 & 0 \\ 0 & 0 & 0 & s_1 \end{pmatrix} \tag{37}$$

where

$$s_1 = \frac{1 - \mathrm{e}^{\mathrm{i}p_2}}{\mathrm{e}^{\mathrm{i}p_1} - 1} \qquad s_2 = \frac{r(\mathrm{e}^{\mathrm{i}p_2} - \mathrm{e}^{\mathrm{i}p_1})}{(1 - \mathrm{e}^{\mathrm{i}p_1})\,[1 + (r-1)\mathrm{e}^{\mathrm{i}p_1}]} \qquad s_3 = \frac{(1-r)\mathrm{e}^{\mathrm{i}p_2} - 1}{1 + (r-1)\mathrm{e}^{\mathrm{i}p_1}}. \tag{38}$$

The matrix $S_{12}(p_1, p_2)$ is obtained from equation (26) in which matrix $\mathbf{b}$ in equation (21) (with $s = 0$) has been used. By inserting equation (37) into equation (36), we find

$$\begin{pmatrix} P_{AA} \\ P_{AB} \\ P_{BA} \\ P_{BB} \end{pmatrix} (\boldsymbol{x}; t|\beta, \boldsymbol{y}, 0) = \begin{pmatrix} a(F_0(t) + F_1(t)) \\ b(F_0(t) + F_1(t)) + cF_2(t) \\ c(F_0(t) + F_3(t)) \\ d(F_0(t) + F_1(t)) \end{pmatrix} \tag{39}$$

in which

$$F_0(t) = \frac{1}{(2\pi)^2} \int \mathrm{e}^{-\epsilon_2 t} \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})}\, \mathrm{d}p_1\, \mathrm{d}p_2 \tag{40}$$

$$F_i(t) = \frac{1}{(2\pi)^2} \int \mathrm{e}^{-\epsilon_2 t} \mathrm{e}^{\mathrm{i}(\tilde{\boldsymbol{p}}\cdot\boldsymbol{x} - \boldsymbol{p}\cdot\boldsymbol{y})} s_i(p_1, p_2)\, \mathrm{d}p_1\, \mathrm{d}p_2 \qquad (i = 1, 2, 3). \tag{41}$$

In the above equations, we have suppressed the $\boldsymbol{x}$ and $\boldsymbol{y}$ dependence of F_i, for simplicity, and $\tilde{\boldsymbol{p}} = (p_2, p_1)$. Now at $t = 0$, the configuration of the system can be one of (A, A), (A, B), (B, A) or (B, B), where the first particle is at site y_1 and the second at y_2, therefore the only acceptable behaviour of $F_i(0)$ $(i = 0, 1, 2, 3)$ is:

$$F_0(0) = \delta_{x_1,y_1}\delta_{x_2,y_2} \qquad F_1(0) = F_2(0) = F_3(0) = 0. \tag{42}$$

$F_0(0)$ is obviously correct (see equation (40)). For the other F_i, first we must set $p_1 \to p_1 + \mathrm{i}\varepsilon$ to avoid the singularity arising from the $\mathrm{e}^{\mathrm{i}p_1} - 1$ term in the denominator of s_1 and s_2 (see [14–17]). In this way one can show that $F_1(0) = 0$. But F_2 and F_3 have another singularity because of the $1 + (r-1)\mathrm{e}^{\mathrm{i}p_1}$ term in the denominator of s_2 and s_3. One can easily show that this singularity can be avoided only when

$$0 \leqslant r < 2 \tag{43}$$

and for this range of interaction rates, we have $F_2(0) = F_3(0) = 0$. Therefore the validity of expansion (36) is restricted to the range (43). At $t \neq 0$, we find

$$F_0(t) = \mathrm{e}^{-2t} \frac{t^{x_1-y_1}}{(x_1-y_1)!} \frac{t^{x_2-y_2}}{(x_2-y_2)!}$$

$$F_1(t) = \mathrm{e}^{-2t} \left[\frac{t^{x_1-y_2+1}}{(x_1-y_2+1)!} - \frac{t^{x_1-y_2}}{(x_1-y_2)!} \right] \sum_{k=0}^{\infty} \frac{t^{x_2-y_1+k}}{(x_2-y_1+k)!}$$

$$F_2(t) = r\mathrm{e}^{-2t} \frac{t^{x_1-y_2}}{(x_1-y_2)!} \sum_{l,k=0}^{\infty} \left[\frac{1}{x_1-y_2+1} - \frac{1}{x_2-y_1+k+l+1} \right] (1-r)^l \frac{t^{x_2-y_1+k+l+1}}{(x_2-y_1+k+l)!}$$

$$F_3(t) = \mathrm{e}^{-2t} \frac{t^{x_1-y_2}}{(x_1-y_2)!} \left[\frac{(1-r)t}{(x_1-y_2+1)!} - 1 \right] \sum_{k=0}^{\infty} (1-r)^k \frac{t^{x_2-y_1+k}}{(x_2-y_1+k)!}. \tag{44}$$

One can now obtain the two-particle conditional probabilities for different initial conditions:

1. If at $t = 0$, the particles $\beta_1 = \beta_2 = A$ were at y_1 and y_2, respectively, we must take $a = 1$ and $b = c = d = 0$. So at $t \neq 0$, we have
$$P_{AA}(\boldsymbol{x}; t|A, A, \boldsymbol{y}; 0) = F_0(t) + F_1(t) \tag{45}$$
and all other P are zero.
2. If $\beta_1 = A$ and $\beta_2 = B$, we must take $b = 1$ and $a = c = d = 0$. Therefore the only nonzero probability is
$$P_{AB}(\boldsymbol{x}; t|A, B, \boldsymbol{y}; 0) = F_0(t) + F_1(t). \tag{46}$$
3. If $\beta_1 = B$ and $\beta_2 = A$, we have $c = 1$ and $a = b = d = 0$. So $P_{AA} = P_{BB} = 0$ and
$$\begin{aligned} P_{AB}(\boldsymbol{x}; t|B, A, \boldsymbol{y}; 0) &= F_2(t) \\ P_{BA}(\boldsymbol{x}; t|B, A, \boldsymbol{y}; 0) &= F_0(t) + F_3(t). \end{aligned} \tag{47}$$
4. And finally, if $\beta_1 = \beta_2 = B$, we have $d = 1$ and $a = b = c = 0$. So the only nonzero probability is
$$P_{BB}(\boldsymbol{x}; t|B, B, \boldsymbol{y}; 0) = F_0(t) + F_1(t). \tag{48}$$
Note that the appearance of the above probabilities is in agreement with our reactions (2).

As another check of our results, it may be interesting to study the long-time behaviour of these probabilities, especially $P_{AB}(\boldsymbol{x}; t|B, A, \boldsymbol{y}; 0)$ which is the only nondiagonal nontrivial case. We expect that if at $t = 0$ we have a B particle at site y_1 and an A particle at site y_2 (with $y_2 > y_1$), we must certainly have two B particles at $t \to \infty$ somewhere at $y_1 \leqslant x_1 < x_2$ and $y_2 \leqslant x_2 < \infty$ sites. In other words, we expect
$$\sum_{x_2=y_2}^{\infty} \sum_{x_1=y_1}^{x_2-1} P_{AB}(\boldsymbol{x}; t \to \infty|B, A, \boldsymbol{y}; 0) \to 1. \tag{49}$$
After some calculations, one can show that
$$\sum_{x_2=y_2}^{\infty} \sum_{x_1=y_1}^{x_2-1} P_{AB}(\boldsymbol{x}; t|B, A, \boldsymbol{y}; 0) = \mathrm{e}^{-2t} \sum_{n=0}^{\infty} [1 - (1-r)^{n+1}][I_{n+y_2-y_1}(2t) + I_{n+y_2-y_1+1}(2t)] \tag{50}$$
where $I_n(x)$ is the nth order Bessel function of the first kind. To obtain the long-time behaviour of (50), one may simply use the following asymptotic form of $I_n(x)$ at $x \to \infty$:
$$I_n(x) \to \frac{\mathrm{e}^x}{\sqrt{2\pi x}} \tag{51}$$
in equation (50). But it is not correct since equation (51) is only valid for $x > n$, but in equation (50) we have a sum over n where for every large definite t, there exists an infinite number of n which are greater than t. (It can be shown that on calculating this limit without noting this point, one finds infinity for equation (50), which is obviously wrong.) To calculate this limit, if one uses the identity $\sum_{n=-\infty}^{\infty} I_n(x) = \mathrm{e}^x$ and takes advantage of the equality $I_n(x) = I_{-n}(x)$, it can be shown that
$$\sum_{n=0}^{\infty} I_{n+k}(x) = \frac{1}{2}\left(\mathrm{e}^x - \sum_{n=-k+1}^{k-1} I_n(x)\right).$$
Therefore
$$\mathrm{e}^{-2t} \sum_{n=0}^{\infty} [1 - (1-r)^{n+1}] I_{n+k}(2t) = \frac{1}{2} - \mathrm{e}^{-2t} \sum_{n=-k+1}^{k-1} I_n(2t) - \mathrm{e}^{-2t} \sum_{n=0}^{\infty} (1-r)^{n+1} I_{n+k}(2t). \tag{52}$$

Now in the second term on the RHS of (52), n is bounded, so equation (51) can be used for it which leads to zero in the $t \to \infty$ limit. For the third term we note that $-1 < 1 - r < 1$ (see equation (43)), so $(1-r)^{n+1} \to 0$ for large n. One can show that this extra $(1-r)^{n+1}$ factor causes the third term on the RHS of (52) to be zero at the $t \to \infty$ limit. Therefore at the $t \to \infty$ limit the RHS of (52) is equal to $1/2$, from which equation (49) is proved.

4. Two-species model with left–right diffusion

In this section we study the range of parameters (reaction rates), which makes the reactions (4) integrable. In this case the master equation is

$$\begin{aligned}\frac{\partial}{\partial t}P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N;t) &= D_R\sum_{i=1}^{N}P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_{i-1},x_i-1,x_{i+1},\ldots,x_N;t)\\ &+ D_L\sum_{i=1}^{N}P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_{i-1},x_i+1,x_{i+1},\ldots,x_N;t)\\ &- N P_{\alpha_1\cdots\alpha_N}(x_1,\ldots,x_N;t)\end{aligned} \tag{53}$$

in which we have used a time scale so that

$$D_R + D_L \equiv 1. \tag{54}$$

The boundary conditions are

$$\begin{aligned}&D_R P_{AB}(x,x) + D_L P_{AB}(x+1,x+1) = r P_{BA}(x,x+1) + (1-s)P_{AB}(x,x+1)\\ &D_R P_{BA}(x,x) + D_L P_{BA}(x+1,x+1) = s P_{AB}(x,x+1) + (1-r)P_{BA}(x,x+1)\\ &D_R P_{\alpha\alpha}(x,x) + D_L P_{\alpha\alpha}(x+1,x+1) = P_{\alpha\alpha}(x,x+1) \qquad (\alpha = A, B).\end{aligned} \tag{55}$$

Note that for $D_L = 0$, equations (53) and (55) reduce to equations (5) and (6), respectively, and for $r = s = 0$, these equations lead to the corresponding ones in [14].

We must proceed along the same steps as in the previous section, which in this case lead to the following relations for energy and boundary conditions:

$$\epsilon_N = \sum_{j=1}^{N}(1 - D_R e^{-ip_j} - D_L e^{ip_j}) \tag{56}$$

and

$$D_R\Psi(\ldots,\zeta,\zeta,\ldots) + D_L\Psi(\ldots,\zeta+1,\zeta+1,\ldots) = \boldsymbol{b}_{k,k+1}\Psi(\ldots,\zeta,\zeta+1,\ldots) \tag{57}$$

where $\mathbf{b}_{k,k+1}$ is defined through (20) with $\mathbf{b}$ in equation (21). If we substitute the coordinate Bethe ansatz (18) in equation (57), the relation between coefficients is like equation (24), but now with the following S-matrix:

$$\mathbf{S}(z_1,z_2) = -(D_R + z_1z_2D_L - z_1\mathbf{b})^{-1}(D_R + z_1z_2D_L - z_2\mathbf{b}). \tag{58}$$

This S-matrix must satisfy the QYBE (28). As in the previous case, there are also 14 equations here that must be solved for r, s and extra D_R parameters (D_L is fixed by D_R through equation (54)). These equations are highly nonlinear and we are not able to solve them exactly, even by using standard programs such as MAPLE. So we restrict ourselves to the cases in which

$$r + s = 1. \tag{59}$$

In this way, we can find the complete set of solutions. We believe that there are no other solutions even if the constraint (59) is removed (we have checked many other cases, but none

satisfied QYBE). The solutions with $r = 0$ or $s = 0$ are not new. They are the known models like the models introduced in (29), or the simple diffusion models introduced in [14] (in which both r and s are zero). There is only one integrable model with $r, s \neq 0$, as follows:

$$\begin{array}{lll} A + \emptyset \xrightarrow{D_R} \emptyset + A & B + \emptyset \xrightarrow{D_R} \emptyset + B & \emptyset + A \xrightarrow{D_L} A + \emptyset \\ \emptyset + B \xrightarrow{D_L} B + \emptyset & B + A \xrightarrow{D_R} A + B & A + B \xrightarrow{D_L} B + A \end{array} \tag{60}$$

in which $D_R = 1 - D_L$. In this way we find a one-parameter family integrable model, whose time-dependent probability can be found by equation (9), with ϵ_N in equation (56), $\mathbf{\Psi}$ is given by (18) and (24), with the S-matrix introduced in (58), and $\mathbf{b}$ in (21).

Note that the reaction–diffusion (60) is the same as the one considered in [18] (equations (4)–(6)), which has been shown equivalent to (after a similarity transformation) the anisotropic version of the spin-1 model introduced by Sutherland [19], with $U_q SU(3)$ symmetry.

It may be interesting to investigate the relation of the p-species models, introduced in section 2, with (P, M) Perk–Schultz quantum chains [20], with Hamiltonian

$$H^{(P,M)} = \sum_{j=1}^{L-1} e_j^{(P,M)} \tag{61}$$

where

$$e_j^{(P,M)} = \frac{q+q^{-1}}{2} - \left[\sum_{\alpha \neq \beta} E_j^{\alpha\beta} E_{j+1}^{\beta\alpha} + \frac{q+q^{-1}}{2} \sum_{\alpha=0}^{N-1} \epsilon_\alpha E_j^{\alpha\alpha} E_{j+1}^{\alpha\alpha} + \frac{q-q^{-1}}{2} \sum_{\alpha \neq \beta} \mathrm{sign}(\alpha - \beta) E_j^{\alpha\alpha} E_{j+1}^{\beta\beta} \right]. \tag{62}$$

In equation (62), L is the number of sites, $N - 1$ is the number of species and the parameters ϵ_α are

$$\epsilon_0 = \epsilon_1 = \cdots = \epsilon_{P-1} = -\epsilon_P = \cdots = -\epsilon_{P+M-1}. \tag{63}$$

It can be shown that $H^{(P,M)}$ is $U_q(SU(P, M))$ invariant [21], and the operators e_j satisfy the Hecke algebra $H_n(q)$ $(n = L - 1)$:

$$e_i e_{i\pm1} e_i - e_i = e_{i\pm1} e_i e_{i\pm1} - e_{i\pm1} \qquad [e_i, e_j] = 0 \qquad |i - j| \geqslant 2 \qquad e_i^2 = (q + q^{-1}) e_i. \tag{64}$$

Now by obtaining the spectrum of (62), it is not difficult to show that the $(N, 0)$ Perk–Schultz model with $\epsilon_\alpha = 1$ and $q + q^{-1} = 1$ is equivalent (by a nonlocal similarity transformation) to our $(N - 1)$-species models when all r_{ij} are equal to 1. For example, in the four-species case, only the last set of allowed parameters in equation (35), where one can choose all r_{ij} to be the same, can be equivalent to the (5, 0) Perk–Schultz model. For other (P, M) models, one cannot tune the parameters to recover the spectrum of our p-species models.

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