A class of solvable reaction–diffusion processes on a Cayley tree

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ABSTRACT

Considering the most general one-species reaction–diffusion processes on a Cayley tree, it has been shown that there exist two integrable models. In the first model, the reactions are the various creation processes, i.e. $\circ \circ \rightarrow \bullet \circ$, $\circ \circ \rightarrow \bullet \bullet$ and $\circ \bullet \rightarrow \bullet \bullet$, and in the second model, only the diffusion process $\bullet \circ \rightarrow \circ \bullet$ exists. For the first model, the probabilities $P_l(m; t)$ of finding $m$ particles on the $l$th shell of the Cayley tree, have been found exactly, and for the second model, the functions $P_l(1; t)$ have been calculated. It has been shown that these are the only integrable models if one restricts consideration to the $L+1$-shell probabilities $P(m_0, m_1, \ldots, m_L; t)$.

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1. Introduction

The integrable reaction–diffusion processes have been investigated by various methods on the one-dimensional lattice. A class of these models are characterized by a master equation with appropriate boundary conditions. These boundary terms, which determine the probabilities at the boundary of the space of the parameters, are chosen such that studying of the various reactions becomes possible via a simple master equation. The basic quantity in these models is the conditional probability $P(\alpha_1, \ldots, \alpha_N, x_1, \ldots, x_N; t | \beta_1, \ldots, \beta_N, y_1, \ldots, y_N; 0)$, which is the probability of finding particles $\alpha_1, \ldots, \alpha_N$ at time $t$ at sites $x_1, \ldots, x_N$, respectively, if at $t = 0$ we have particles $\beta_1, \ldots, \beta_N$ at sites $y_1, \ldots, y_N$, respectively [1–6].

Another class of models are those which are solvable through the empty interval method. In these models, the main quantity, in the most general case, is $E_{k,n}(t)$, which is the probability that $n$ consecutive sites, starting from the site $k$, are empty. Several examples have been investigated by this method [7–13].

The crucial property which governs whether the above mentioned cases are analytically solvable is the dimension of the lattice which particles move on. The one-dimensional lattice is clearly the simplest case.

Considering lattices of higher dimension in studying the integrable models is obviously a great improvement in theoretical physics. One of the important examples in this area is that of the Cayley tree. A Cayley tree is a connected cycle-free graph where each site is connected to $z$ neighbor sites. $z$ is called the coordination number. The Cayley tree of coordination number $z$ may be constructed by starting from a single central node (called the root of the lattice) at shell $l = 0$, which is connected to $z$ neighbors at shell $l = 1$. Each of the nodes in shell $l > 0$ is connected to $(z − 1)$ nodes in shell $l + 1$. This construction may stop at shell $l = L$, or continue indefinitely (Fig. 1). The interior of an infinite Cayley tree is called the Bethe lattice. Due to the distinctive topological structure of the Cayley tree, the reaction–diffusion processes on this graph may be integrable.

The diffusion-controlled process of cluster growth, introduced by Witten and Sander [14], has been studied on the Cayley tree in Ref. [15], and in Ref. [16], the two-particle annihilation reaction for immobile reactant has been studied on the Bethe lattice. Diffusion-limited coalescence, $A + A \rightarrow A$, and annihilation, $A + A \rightarrow 0$ [17], and random sequential adsorption [18] have also been studied on the Cayley tree. Also the reaction–diffusion processes on the Cayley tree, solvable through the empty interval method, have been studied in Ref. [19].

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The present paper is devoted to the study of some integrable reaction–diffusion processes on the Cayley tree. Denoting the number of particles on the $l$th shell by $m_l$, we seek the situations in which the probability $P(m_0, m_1, m_2, \ldots, m_L; t)$ can be calculated exactly. $l_{\text{max}} = L$ is the last shell of the Cayley tree. By considering the most general reactions on the Cayley tree in Section 2, it is shown that we must restrict ourselves to three distinct creation reactions so that a subclass of $L + 1$-shell probabilities $P(m_0, m_1, \ldots, m_L; t)$, i.e. $P_l(m; t) \equiv P(0, 0, \ldots, 0, m_l = m, 0, \ldots, 0; t)$, becomes solvable. The exact solution for $P_l(m; t)$ is obtained in Section 3. Finally in the concluding section it is shown that the diffusion process can also lead to an integrable model, if one restricts consideration to one-particle probabilities $P_l(1; t)$, and if an extra trapping reaction exists at the central node. An ideal spherical trap surrounded by a swarm of Brownian particles is a fundamental model which was first presented by von Smoluchowski [20], and has been generalized to a mobile trap in Ref. [21]. Also the energy transfer process in the dendrimer supermolecule on the Cayley tree with a central trap has been discussed in Ref. [22]. These two models are the only integrable models in this context.

It must be added that the procedure introduced in this paper can be easily extended to situations in which the number of occupied shells is greater than 1, but there must exist at least one empty shell between any two of them.

2. The integrable models

The most general reactions of single-species models with nearest-neighbor interactions are

\begin{align*}
1: \circ \circ & \rightarrow \bullet \circ, \quad r_1 \\
2: \circ \circ & \rightarrow \bullet \bullet, \quad r_2 \\
3: \circ \bullet & \rightarrow \bullet \bullet, \quad r_3 \\
4: \circ \bullet & \rightarrow \circ \bullet, \quad r_4 \\
5: \bullet \circ & \rightarrow \circ \circ, \quad r_5 \\
6: \bullet \circ & \rightarrow \bullet \bullet, \quad r_6 \\
7: \bullet \bullet & \rightarrow \circ \bullet, \quad r_7
\end{align*}

where an empty (occupied) site is denoted by $\circ$ ($\bullet$). The $r_i$ are reaction rates and there is no distinction between left and right. Our main goal is to find the situations which lead to integrable models. By integrability, we mean the possibility of the exact calculation of probabilities $P(m_0, m_1, \ldots; t)$.

The necessary condition for achieving this goal is that the occupation numbers of shells (the numbers of occupied sites of every shell) must be the only parameters needed to characterize the configurations. Clearly this is not the case if two adjacent shells are occupied. For example consider $P(0, 1, 2; t)$ and the reaction (1) of Eq. (1). In Figs. 2 and 3, the source terms of two
different configurations (a) and (b), with same occupation numbers (0, 1, 2), are shown. As is seen, the configuration (a) has two source terms, while the configuration (b) has three. The number behind each configuration is its multiplicity, i.e. the number of ways in which this configuration can lead to the desired state. This shows that if two adjacent shells are occupied, it is not possible to write the same evolution equation for different configurations of a given occupation numbers. Therefore, we only consider the situations in which there is only one non-zero occupation number, i.e. \( m_l = m \delta_{il} \). As mentioned earlier, it is possible to extend our procedure to situations in which there is at least one empty shell between any two occupied shells.

Considering the probabilities \( P_l(m; t) = P(0, 0, \ldots, 0, m_l = m, 0, \ldots, 0; t) \), we must check whether all the reactions of Eq. (1) are acceptable or not. By the term acceptable, we mean having two properties, as follows. First, the determination of the occupation number \( m \) is sufficient for having a unique evolution equation, irrespective of the particles’ distribution. Second, all the terms of the evolution equation are expressible in terms of the \( P_k(n; t) \). Now it can be seen that this is not the case for reactions (4)–(7) of Eq. (1). This is because in all these cases, the source terms of the \( P_l(m; t) \) are two-shell probabilities \( P(m_{l-1}, m_l; t) \) and \( P(m_l, m_{l+1}; t) \), which cannot be expressed in terms of the \( P_k(n; t) \). For these reactions, the master equations are

\[
\begin{align*}
\frac{\partial}{\partial t} P_l(m; t) &= a_4 P_l(m_{l-1} = 1, m_l = m - 1; t) + b_4 P_l(m_l = m - 1, m_{l+1} = 1; t) - s_4 P_l(m; t) \quad \text{(for } r = r_4), \\
\frac{\partial}{\partial t} P_l(m; t) &= a_5 P_l(m_{l-1} = 1, m_l = m; t) + b_5 P_l(m_l = m, m_{l+1} = 1; t) + c_5 P_l(m + 1; t) - s_5 P_l(m; t) \quad \text{(for } r = r_5), \\
\frac{\partial}{\partial t} P_l(m; t) &= a_6 P_l(m_{l-1} = 1, m_l = m + 1; t) + b_6 P_l(m_l = m + 1, m_{l+1} = 1; t) \quad \text{(for } r = r_6), \\
\frac{\partial}{\partial t} P_l(m; t) &= a_7 P_l(m_{l-1} = 1, m_l = m; t) + b_7 P_l(m_l = m, m_{l+1} = 1; t) \quad \text{(for } r = r_7),
\end{align*}
\]

respectively. The parameters \( a_i, b_i, c_i \) and \( s_i \) are some constants. The case of \( m = 1 \) is an exception which will be discussed in Section 4.

So the integrable model, through the \( P_l(m; t) \) probabilities, is a model in which the allowed reactions are reactions (1)–(3) of Eq. (1). The evolution equation for \( P_l(m; t) \) on a Cayley tree with coordination number \( z \) and \( L + 1 \) shells then becomes (for \( l = 0, 1, 2, \ldots, L - 1 \))

\[
\frac{\partial}{\partial t} P_l(m; t) = (n_l - m + 1)zr_1 P_l(m - 1; t) - \left[ 2 \left( \sum_{r=1}^{L} n_r - mz \right) r_1 + \left( \sum_{r=1}^{L} n_r - mz \right) r_2 + mr_3 \right] P_l(m; t).
\]

In the above equation

\[
n_l = \begin{cases} 
(z - 1)^{l-1} & \text{for } l \geq 1 \\
1 & \text{for } l = 0
\end{cases}
\]

is the number of sites of the \( l \)th shell. The first term in the right-hand site of Eq. (6) is the source term of reaction (1), and \( 2(\sum_{r=1}^{L} n_r - mz)r_1 P_l(m; t) \) is its sink term. This is because \( \sum_{r=1}^{L} n_r - mz \) is the number of empty pairs \((oo)\) of a Cayley tree with \( m \) particles on shell \( l \), where each of them can change to either \( oo \) or \( oo \) with rate \( r_1 \). The reaction (2) has no source term for \( P_l(m; t) \), and its sink term is clearly \( (\sum_{r=1}^{L} n_r - mz)r_2 P_l(m; t) \). Finally the reaction (3) does not have a source term, and its sink term is \( mr_3 P_l(m; t) \) because each of the neighbors of each particle of the \( l \)th shell can be changed via the \( oo \to oo \) reaction.

For \( l = L \), since there is no upper shell, the number of neighboring sites of each occupied site is 1, instead of \( z \). Therefore for \( P_l(m; t) \), the evolution equation is same as Eq. (6), when \( z \) is replaced by 1.

3. Solutions of the master equation

In this section we try to solve the master equation

\[
\frac{\partial}{\partial t} P_l(m; t) = (n_l - m + 1)zr_1 P_l(m - 1; t) - [(r_3 - r_2 - 2r_1)mz + (2r_1 + r_2)N]P_l(m; t) \quad (l < L),
\]

with

\[
N \equiv \sum_{r=1}^{L} n_r,
\]

for the two cases of \( r_3 - r_2 - 2r_1 \neq 0 \) and \( r_3 - r_2 - 2r_1 = 0 \). For \( l = L \), we must set \( z = 1 \) in Eq. (8).
3.1. The case of \( r_3 \neq r_2 + 2r_1 \)

To solve Eq. (8), we use a recursive method. We first consider the case of \( m = 0 \), where Eq. (8) is reduced to

\[
\frac{\partial}{\partial t} P_l(0; t) = -N(2r_1 + r_2) P_l(0; t),
\]

with the solution

\[
P_l(0; t) = P_l(0)e^{-N(2r_1 + r_2)t}.
\]

\( P_l(0) \equiv P_l(0; t = 0) \) is the probability of finding no particle in shell \( l \) at \( t = 0 \). Inserting Eq. (11) in the \( m = 1 \) case of Eq. (8) results in \( P_l(1; t) \) as follows:

\[
P_l(1; t) = \left[ P_l(1) - \frac{n_t r_1 P_l(0)}{r_3 - r_2 - 2r_1} \right] e^{-[\xi(t_0 - r_2 - 2r_1)] + N(2r_1 + r_2)t} + \frac{n_t r_1 P_l(0)}{r_3 - r_2 - 2r_1} e^{-N(2r_1 + r_2)t}.
\]

Continuing this method, one can deduce the following general expression for \( P_l(m; t) \):

\[
P_l(m; t) = \sum_{k=0}^{m} \sum_{j=0}^{k} \frac{(n_l - j)! (n_t - j)!}{(n_l - m)! (m - k)!} \left( \frac{r_1}{r_3 - r_2 - 2r_1} \right)^{m-j} (-1)^{k-j} P_l(j) e^{-[\xi(t_0 - r_2 - 2r_1)] + N(2r_1 + r_2)t} (l < L).
\]

In which, as we will show, \( P_l(j) \equiv P_l(j; t = 0) \).

It can be seen that for \( m = 0 \) and \( m = 1 \), Eq. (13) leads to Eqs. (11) and (12), respectively. To prove that Eq. (13) is the solution of Eq. (8), we insert it in Eq. (8). The summations in the left-hand side and in the second term of the right-hand side of Eq. (8) are both \( \sum_{k=0}^{m} \sum_{j=0}^{k} \). If we write them as \( \sum_{j=0}^{n_t} + \sum_{j=0}^{n_t-1} \sum_{j=0}^{k} \), then it can be seen that the \( \sum_{j=0}^{n_t} \) terms in both sides are the same, and therefore they cancel. So in all three terms of Eq. (8), the summations have the same form, \( \sum_{j=0}^{n_t} \sum_{k=0}^{m} \), and after some simple calculations, it can be shown that the remaining terms are cancelled, which proves that the expression (13) satisfies the master equation (8). Note that because of the \((n_l - m)!\) factor in the denominator of Eq. (13), \( P_l(m; t) \) satisfies

\[
P_l(m > n_l; t) = 0,
\]

which shows the correct behavior of Eq. (13).

It is also necessary to prove the physical interpretation of \( P_l(j) \) as \( P_l(j; t = 0) \). To see this, we consider Eq. (13) at \( t = 0 \):

\[
P_l(m; t = 0) = \sum_{j=0}^{m} \sum_{k=0}^{m} \frac{r_1}{r_3 - r_2 - 2r_1}^{m-j} \frac{(n_l - j)!}{(n_l - m)!} \frac{P_l(j)}{(m - k)!} (-1)^{k-j} j^{m-j}.
\]

In which we use the equality

\[
\sum_{k=0}^{m} \sum_{j=0}^{k} A(j, k) = \sum_{j=0}^{m} \sum_{k=j}^{m} A(j, k).
\]

Using \( k' = k - j \), Eq. (15) becomes

\[
P_l(m; t = 0) = \sum_{j=0}^{m} \left( \frac{r_1}{r_3 - r_2 - 2r_1} \right)^{m-j} \frac{(n_l - j)!}{(n_l - m)!} P_l(j) \frac{(-1)^{k'}}{k!(m-j-k')!}.
\]

From binomial expansion,

\[
(a - b)^n = \sum_{k'=0}^{n} (-1)^{k'} \frac{n!}{k!(n-k)!} a^{n-k} b^k,
\]

one finds for \( a = b \)

\[
0 = n! a^n \sum_{k'=0}^{n} (-1)^{k'} \frac{1}{k!(n-k)!}.
\]

So the last summation of Eq. (17) is zero for all \( m - j \neq 0 \), or \( j = 0, 1, \ldots, m - 1 \). The only remaining term is \( j = m \), which results in

\[
P_l(m; t = 0) = P_l(m).
\]

This completes the proof of Eq. (13) as the exact solution of the master equation (8), with the \( P_l(j) \) as the initial values of the probabilities. The probability \( P_l(m; t) \) is found from (13), by taking \( l = L \) and \( z = 1 \).

Eq. (13) gives the probability of finding \( m \) particles at time \( t \) on shell \( l \), when all other shells are empty, if we begin with any number of particles on shell \( l \) at \( t = 0 \). Of course for a specific initial condition, i.e. \( P_l(j; t = 0) = \delta_{j,0} \), only one term of the summation \( \sum_{j=0}^{k} \) survives.
3.2. The case of \( r_3 = r_2 + 2r_1 \)

For the case of \( r_3 = r_2 + 2r_1 \), the master equation (8) becomes

\[
\frac{\partial}{\partial t} P_l(m; t) = (n_l - m + 1)zr_3P_l(m - 1; t) - Nr_3P_l(m; t) \quad (l < L).
\]  

(21)

Using the method of the previous case, the solution of the above equation is found to be

\[
P_l(m; t) = e^{-Nr_3t} \sum_{j=0}^{m} \frac{(n_l - j)!}{(m - j)!(n_l - m)!} P_j(r_3zt)^{m-j} \quad (l < L).
\]

(22)

It can be easily shown that the solution (22) satisfies (21) and has the desired properties \( P_l(m > n_l; t) = 0 \) and \( P_l(m; t = 0) = P_l(m) \). For \( l = L \), the solution is found from Eq. (22), by taking \( l = L \) and \( z = 1 \).

4. Conclusion

To study the integrable reaction–diffusion processes on lattices of more than one dimension, the most general interactions (1) have been considered on a Cayley tree with coordination number \( z \). It has been shown that among the probability functions, the probabilities \( P_l(m; t) \) are independent of the distribution of particles on various shells, and may lead to integrable models if we consider two situations. The first one is that of the creation reactions (1)–(3) of Eq. (1), with master equation (6). The \( P_l(m; t) \) for the two cases \( r_3 \neq r_2 + 2r_1 \) and \( r_3 = r_2 + 2r_1 \) have been considered in Section 3, with the final exact results (13) and (22), respectively.

As is clear from Eqs. (2)–(5), in the case of \( m = 1 \), the master equations (3)–(5) still contain the two-shell probabilities, but for the diffusion process with \( r = r_4 \), only the one-shell probabilities (i.e. one-point functions) appear in Eq. (2), which may lead to an integrable model.

The master equation of \( P_l(1; t) \), with \( l > 1 \), for a diffusion process on a Cayley tree with coordination number \( z \) is

\[
\frac{\partial}{\partial t} P_l(1; t) = (z - 1)P_{l-1}(1; t) + P_{l+1}(1; t) - zP_l(1; t),
\]

in which the diffusion rate \( r_4 \) has been absorbed in the rescaling of time \( t \). The evolution equations for \( P_0(1; t) \) and \( P_l(1; t) \) are

\[
\frac{\partial}{\partial t} P_0(1; t) = P_1(1; t) - zP_0(1; t),
\]

(24)

\[
\frac{\partial}{\partial t} P_l(1; t) = zP_0(1; t) + P_2(1; t) - zP_l(1; t),
\]

(25)

respectively. These equations take a form similar to that of Eq. (23), provided one defines

\[
P_{-1}(1; t) := 0,
\]

(26)

\[
P_0(1; t) := 0.
\]

(27)

The first boundary condition is trivially satisfied, since the \( P_l(m; t) \) have been defined for \( l \geq 0 \). But the second one indicates a trapped reaction at the origin. So Eq. (23), with arbitrary \( l \), defines an integrable model on a Cayley tree if the particles have a diffusion process, and if there exists a trap at the root of the lattice. For when the reactions are the coalescence \( A + A \rightarrow A \) and annihilation \( A + A \rightarrow 0 \), the density of particles in shell \( l \), i.e. \( \rho_l(t) \), has been calculated in Ref. [17] for the same situation, that is a trap at the root of a Cayley tree.

It can be shown that the solution of master equation (23) with boundary condition (27) is

\[
P_l(1; t) = (z - 1)^{(l-\theta_0)/2} \left[ l_{\theta_0-\theta_0}(2(2 - 1)^{1/2} t) - l_{\theta_0+\theta_0}(2(2 - 1)^{1/2} t) \right] e^{-zt},
\]

(28)

in which \( l_{\theta} \) is the nth-order modified Bessel function.

Finally it must be added that there remains one more case which may lead to an integrable model. Looking at Eqs. (2)–(5), it is clear that if one takes \( m = 0 \), only the master equation (3) leads to an equation which only consists of one-point functions, i.e.

\[
\frac{\partial}{\partial t} P_l(0; t) = a_lP_{l-1}(1; t) + b_lP_{l+1}(1; t) + c_lP_l(1; t) - s_lP_l(0; t).
\]

(29)

It can be shown that \( s_l = 0 \). But the point is that the determination of the \( P_l(0; t) \) depends on the evaluation of the \( P_l(1; t) \), which cannot be calculated. This is because the master equation of the \( P_l(1; t) \) contains the two-point probabilities \( P(1, 1; t) \) and therefore is not closed. Therefore the two models considered are the only cases which can be exactly solved.
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