Autonomous models solvable through the full interval method

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Abstract

The most general exclusion single species one dimensional reaction-diffusion models with nearest-neighbor interactions which are both autonomous and can be solved exactly through full interval method are introduced. Using a generating function method, the general solution for, F_n , the probability that n consecutive sites be full, is obtained. Some other correlation functions of number operators at nonadjacent sites are also explicitly obtained. It is shown that for a special choice of initial conditions some correlation functions of number operators called full intervals remain uncorrelated.

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1 Introduction

Most of the analytical studies on non-equilibrium statistical models belong to the low-dimensional (specially one dimensional) models [1–13]. Analyzing one dimensional models, which are usually easier to investigate, helps us gaining knowledge on systems far from equilibrium. One of the techniques used to obtain exact results is the empty interval method (EIM), or its equivalent the full interval method (FIM). Among other things, it has been used to analyze the one dimensional dynamics of diffusion-limited coalescence [14-17]. In these, one dimensional diffusion-limited processes have been studied using EIM. There, some of the reaction rates have been taken infinite, and the models have been worked out on continuum. For the cases of finite reaction-rates, some approximate solutions have been obtained. Using this method E_n (the probability that n consecutive sites be empty) has been calculated. (Alternatively, F_n is the probability that n consecutive sites be full.) This method has been used to study a reaction-diffusion process with three-site interactions [18]. EIM has been also generalized to study the kinetics of the q-state one dimensional Potts model in the zero-temperature limit [19]. In [20], all the one dimensional reactiondiffusion models with nearest neighbor interactions which can be exactly solved by EIM have been found and studied. Conditions have been obtained for the systems with finite reaction rates to be solvable via EIM, and then the equations of EIM have been solved. There solvability means that the evolution equation for E_n be closed. It turned out there, that certain relations between the reaction rates are needed, so that the system is solvable via EIM. When these conditions between reaction rates are met, the time derivative of E_n 's would be linear combinations of E_n 's. It was shown that if certain reactions are absent, namely reactions that produce particles in two adjacent empty sites, the coefficients of the empty intervals in the evolution equation of the empty intervals are *n*-independent, so that the evolution equation can be easily solved. The criteria for solvability, and the solution of the empty-interval equation were generalized to cases of multi-species systems and multi-site interactions in [21-23]. In [24], models were studied which were solvable through EIM, but did include interaction which produce particles in two adjacent empty sites. There these models were investigated in continuum, although some terms in the evolution equation were missed, as will be discussed in the present paper. In [25], conventional EIM has been extended to a more generalized form. Using this extended version, a model has been studied which can not be solved by conventional EIM. Recently, the coagulation-diffusion process on a one dimensional chain has been studied using the empty-interval method [26]. There the behavior of the time-dependent double-empty-interval probability has been studied. In [27], the exact two-time correlation and response functions for a one dimensional coagulation-diffusion process has been studied using EIM.

In [28], a ten-parameter family of reaction-diffusion processes was introduced for which the evolution equation of n-point functions contains only n- or lesspoint functions. We call such systems autonomous. The expectation value of the particle-number in each site has been obtained exactly for these models. In order to be an autonomous model there should be some constraints on the reaction rates.

Here we study the most general exclusion single species one dimensional reaction-diffusion model with nearest-neighbor interactions, which can be solved exactly through the full interval method, and is autonomous. The reaction rates corresponding to these two models apart from corrections to [24], here lattice models are studied, while in [24] such models on continuum were investigated. The change from the empty interval to the full interval is, of course, not important; as a simple interchange of particles and holes would do that. The scheme of the paper is as follows. In Section 2, the most general exclusion single species one dimensional reaction-diffusion models with nearest-neighbor interactions are introduced, which are autonomous and can be solved exactly through FIM. In Section 3, the evolution equation for the full interval probabilities, F_n 's are obtained. In section 4, the steady state solutions for these probabilities are obtained, and then using a generating function method, the general solution for F_n 's is calculated. Correlation functions of number operators at nonadjacent sites are obtained in section 5. Finally, in section 6 some correlation functions of number operators are explicitly calculated for some special choice of initial conditions. These are probabilities of some disjoint parts of the lattice be full.

2 Full interval and autonomy

Consider a one dimensional lattice, any site of which is either occupied by a single particle or empty, and assume that the reactions, as well as the state of the system, are translationally invariant. Implicit in this, is that the lattice has no boundaries. But the lattice can still be finite, if it is circular. Defining F_n as the probability that n consecutive sites be full

$$F_n := P(\overbrace{\bullet \bullet \cdots \bullet}^{\frown}), \tag{1}$$

where an empty (occupied) site is denoted by by \circ (•), it is found (for example similar to [24]), that the most general single species nearest-neighbor interactions for which the evolution equations governing F_n 's are closed are

$$\circ \bullet \to \begin{cases} \circ \circ, & q_1 \\ \bullet \circ, & r_1 \end{cases},$$

$$\bullet \circ \to \begin{cases} \circ \circ, & q_2 \\ \circ \bullet, & r_2 \end{cases},$$

$$\circ \circ \to \begin{cases} \bullet \circ, & r_1 \\ \circ \bullet, & r_2 \end{cases},$$

$$\bullet \bullet \to \begin{cases} \bullet \circ, & w_1 \\ \circ \bullet, & w_2 \end{cases},$$

$$\circ \circ, & w \end{cases}$$

$$(2)$$

where $r_1, r_2, q_1, q_2, w, w_1$ and w_2 are reaction rates. Then the Hamiltonian for a two site interaction for models solvable through FIM is

$$H = \begin{pmatrix} -r_1 - r_2 & q_1 & q_2 & w \\ r_2 & -q_1 - r_1 & r_2 & w_2 \\ r_1 & r_1 & -q_1 - r_1 & w_1 \\ 0 & 0 & 0 & -w - w_1 - w_2 \end{pmatrix}.$$
 (3)

The autonomy criteria leads to two more constraints ([28], for example)

$$r_1 + q_1 = w_1 + w,$$

$$r_2 + q_2 = w_2 + w.$$
(4)

So an autonomous model solvable through FIM has five free parameters.

3 The full interval evolution

The full interval equation is

$$\frac{\mathrm{d}F_n}{\mathrm{d}t} = (r_1 + r_2) \left(F_{n-1} + F_{n+1} - 2F_n\right) - (q_1 + q_2) \left(F_n - F_{n+1}\right) - (n-1) \left(w_1 + w_2 + w\right) F_n - \left(w_1 + w_2 + 2w\right) F_{n+1},$$
(5)

where

$$F_0 := 1.$$
 (6)

The difference of this with what obtained in [24], apart from the obvious interchange of particles and vacancies, is that the last term had been missed in [24]. Using (4), it is seen that the coefficient of F_{n+1} in the right-hand side of (5) vanishes. So,

$$\frac{\mathrm{d}F_n}{\mathrm{d}t} = (r_1 + r_2) F_{n-1} - \left[2 \left(r_1 + r_2\right) + q_1 + q_2 + (n-1) \left(w_1 + w_2 + w\right)\right] F_n.$$
(7)

Rescaling the time by $(w_1 + w_2 + w)$:

$$\tilde{t} := (w_1 + w_2 + w) t,$$
(8)

the evolution equation becomes

$$\frac{\mathrm{d}F_n}{\mathrm{d}\tilde{t}} = b\,F_{n-1} - (a+n-1)\,F_n,\tag{9}$$

where

$$a := \frac{2(r_1 + r_2) + q_1 + q_2}{w + w_1 + w_2},$$

$$b := \frac{r_1 + r_2}{w + w_1 + w_2}.$$
 (10)

Equation (4), and the fact that the rates are nonegative guarantee that $(w_1 + w_2 + w)$ is positive, unless all of the rates are zero. These also show that

$$a \ge 1 + b,\tag{11}$$

$$b \ge 0. \tag{12}$$

From now on, the rescaled time \tilde{t} is denoted by t, so that the evolution equation is written as

$$\dot{F}_n = b F_{n-1} - (a+n-1) F_n, \tag{13}$$

where dot means differentiation with respect to the rescaled time.

4 The general solution for the full interval

Let's first consider the large time values for F_n or the steady state solution. Denoting the time independent equation for the full interval by F_n^{st} , one has

$$F_n^{\rm st} = \frac{b}{a+n-1} F_{n-1}^{\rm st},$$
 (14)

which combined with (6) results in

$$F_n^{\rm st} = \frac{b^n \, \Gamma(a)}{\Gamma(a+n)}.\tag{15}$$

The general solution to (13) is of the form

$$F_n(t) = F_n^{\rm st} + \sum_{m=1}^n c_{n\,m} \, \exp[-(a+m-1)\,t],\tag{16}$$

where $c_{n\,m}$'s are constants. Putting (16) in (13), one arrives at

$$(n-m) c_{n m} = b c_{n-1 m}, \qquad m < n.$$
(17)

This allows one to determine $c_{n\,m}$'s in terms of $c_{m\,m}$'s, which are denoted by d_m :

$$c_{n\,m} = \frac{b^{n-m}}{(n-m)!} c_{m\,m},$$

=: $\frac{b^{n-m}}{(n-m)!} d_m.$ (18)

So,

$$F_n(t) = F_n^{\text{st}} + \sum_{m=1}^n \frac{b^{n-m}}{(n-m)!} d_m \exp[-(a+m-1)t],$$
(19)

showing that the (largest) relaxation time τ is obtained from

$$\tau = \frac{1}{a}.$$
 (20)

The constants d_m are to be obtained from the initial conditions. One way is to define the generating functions G and G^{st} through

$$G := \sum_{n=0}^{\infty} F_n(0) x^n,$$

$$G^{\text{st}} := \sum_{n=0}^{\infty} F_n^{\text{st}} x^n.$$
(21)

Using these and (19),

$$G(x) = G^{\text{st}}(x) + \sum_{n=0}^{\infty} \sum_{m=1}^{n} \frac{b^{n-m}}{(n-m)!} d_m x^n,$$

$$= G^{\text{st}}(x) + \sum_{m=1}^{\infty} \sum_{n=m}^{\infty} \frac{b^{n-m}}{(n-m)!} d_m x^n,$$

$$= G^{\text{st}}(x) + \sum_{m=1}^{\infty} \left(\frac{\partial}{\partial b}\right)^m \sum_{n=0}^{\infty} \frac{b^n}{n!} d_m x^n,$$

$$= G^{\text{st}}(x) + \sum_{m=1}^{\infty} d_m \left(\frac{\partial}{\partial b}\right)^m \exp(bx),$$

$$= G^{\text{st}}(x) + \exp(bx) \sum_{m=1}^{\infty} d_m x^m.$$
(22)

So,

$$\sum_{m=1}^{\infty} d_m x^m = \exp(-b x) [G(x) - G^{\rm st}(x)], \qquad (23)$$

which results in

$$d_m = \sum_{k=0}^{m-1} \frac{(-b)^k}{k!} \left[F_{m-k}(0) - \frac{b^{m-k} \Gamma(a)}{\Gamma(a+m-k)} \right].$$
 (24)

For example, the occupation probability of any site is

$$F_1(t) = \frac{b}{a} + \left[F_1(0) - \frac{b}{a}\right] \exp(-at).$$
 (25)

5 Correlation functions of number operators at nonadjacent site

Denoting the number operator in the site i by n_i , it is seen that

$$\langle \dot{n}_i \rangle = b - a \, \langle n_i \rangle. \tag{26}$$

This is in fact the same as the evolution equation for F_1 , as it should be. The solution to (26) is

$$\langle n_i \rangle(t) = \langle n_i \rangle(0) \exp(-at) + \frac{b}{a} \left[1 - \exp(-at)\right].$$
(27)

Defining the correlation $C_{i_1\cdots i_k}$ as

$$C_{i_0\cdots i_k} := \langle n_{i_0}\cdots n_{i_k} \rangle, \tag{28}$$

where no two indices are adjacent, it is seen that

$$\dot{C}_{i_0\cdots i_k} = b \sum_{j=0}^k C_{i_0\cdots \hat{i_j}\cdots i_k} - (k+1) a C_{i_0\cdots i_k},$$
(29)

where \hat{i} means that the index *i* has been omitted.

A simple change of variable makes the above equations simpler. Defining

$$\tilde{C}_{i_0\cdots i_k} := \left\langle \left(n_{i_0} - \frac{b}{a} \right) \cdots \left(n_{i_k} - \frac{b}{a} \right) \right\rangle, \tag{30}$$

(again for the case no two indices are adjacent) one arrives at

$$\dot{\tilde{C}}_{i_0\cdots i_k} = -(k+1) \, a \, \tilde{C}_{i_0\cdots i_k}. \tag{31}$$

The so called connected correlations \tilde{C}^c are defined inductively through

$$\tilde{C}_i =: \tilde{C}_i^{\rm c}, \tag{32}$$

$$\tilde{C}_{i_0\cdots i_k} =: \sum_{\mathcal{P}} \tilde{C}^{\mathbf{c}}_{\mathcal{P}_1(i_0\cdots i_k)}\cdots \tilde{C}^{\mathbf{c}}_{\mathcal{P}_\alpha(i_0\cdots i_k)},\tag{33}$$

where the summation runs over all partitions \mathcal{P} of $(i_0 \cdots i_k)$. Such a partition divides the indices $(i_0 \cdots i_k)$ into α parts, where the β 'th part is denoted by $\mathcal{P}_{\beta}(i_0 \cdots i_k)$. A simple induction shows that

$$\tilde{C}^{c}_{i_0\cdots i_k} = -(k+1) \, a \, \tilde{C}^{c}_{i_0\cdots i_k}. \tag{34}$$

Another induction shows that for k > 0, adding a constant to any of n_{i_j} 's does not change the connected correlations. The reason is that, denoting the correlations and connected correlations corresponding to $(n_{i_k} + \Delta)$ by a superscript Δ , one has

$$\tilde{C}^{\Delta c}_{i_0 \cdots i_k} = \tilde{C}^{\Delta}_{i_0 \cdots i_k} - \tilde{C}^{\Delta}_{i_0 \cdots i_{k-1}} \tilde{C}^{\Delta}_{i_k} + R,$$
(35)

where R contains terms in which the index i_k enters connected correlations of (m + 1) operators, where m is positive but less than k. Assuming that the independence of the connected correlations of (m + 1) operators is true for m positive and less than k, it is seen that R does not depend on Δ . The sum of the first two terms of the right hand side is also obviously independent of Δ . So

the left hand side is independent of Δ as well. To complete the induction, one should prove that the connected correlation of two number operators does not change upon adding a constant term to each of them. This is obvious since in that case, R in the right of (35) is zero.

In particular, one arrives at

$$C_{i_0\cdots i_k}^{\rm c} = \tilde{C}_{i_0\cdots i_k}^{\rm c}, \qquad k > 0,$$
 (36)

showing that

$$C_{i_0\cdots i_k}^{\mathbf{c}}(t) = C_{i_0\cdots i_k}^{\mathbf{c}}(0) \, \exp[-(k+1)\,a\,t], \qquad k > 0.$$
(37)

The simplest example of this, is the connected two point function:

$$(\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle)(t) = (\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle)(0) \exp(-2 a t), \quad |j - i| > 1.$$
(38)

To consider correlations with possibly adjacent sites, let us first obtain the evolution equation for the full interval, without the assumption of translational invariance. Defining F_{ij} as the probability that the sites beginning from *i* ending in *j* are full, one arrives at

$$\dot{F}_{ij} = b_1 F_{ij-1} + b_2 F_{i+1j} - (a+j-i) F_{ij}, \qquad (39)$$

where

$$b_1 := \frac{r_1}{w + w_1 + w_2},$$

$$b_2 := \frac{r_2}{w + w_1 + w_2}.$$
(40)

Then, reassuming translational invariance define D_{ℓ} as

$$D_{\boldsymbol{\ell}} := \left\langle \prod_{j=0}^{k} \left(\prod_{m=1}^{\ell_{2j}} n_{\ell_0 + \dots + \ell_{2j-1} + m} \right) \right\rangle, \tag{41}$$

where

$$\boldsymbol{\ell} := (\ell_0, \dots, \ell_{2k}), \tag{42}$$

and ℓ_j 's are positive integers. This is the probability that ℓ_0 consecutive sites beginning from 1 be full, ℓ_2 consecutive sites beginning from $(\ell_0 + \ell_1 + 1)$ be full, and so on. In the special case k = 0, this correlation is the same as the full interval:

$$D_{\ell} = F_{\ell}.\tag{43}$$

In the special case that all ℓ_j 's with even j are one, D is reduced to the (k+1)-point function with nonadjacent sites:

$$D_{1,\ell_1\,1,\ldots,\ell_{2\,k-1},1} = C_{i_0\cdots i_k},\tag{44}$$

$$i_{m+1} - i_m = \ell_{2\,m+1} + 1. \tag{45}$$

Using (39) and (41), it is then seen that

$$\dot{D}_{\boldsymbol{\ell}} = \sum_{m=0}^{k} [b_2 D_{\boldsymbol{\ell}-\boldsymbol{e}_{2\,m}+\boldsymbol{e}_{2\,m-1}} + b_1 D_{\boldsymbol{\ell}-\boldsymbol{e}_{2\,m}+\boldsymbol{e}_{2\,m+1}} - (a + \ell_{2\,m} - 1) D_{\boldsymbol{\ell}}], \quad (46)$$

where e_m is a (2k+1)-tuple, the only nonzero component of which is the *m*-th component being equal to one, and e_{-1} and e_{2k+1} are zero.

A special case is the two-point function. For nonadjacent sites, one use

$$\dot{C}_{ij} = b \left(C_i + C_j \right) - 2 a C_{ij},$$
(47)

the solution to which is

$$C_{ij}(t) = \langle n_i \, n_j \rangle(0) \, \exp(-2 \, a \, t) + \frac{b^2}{a^2} \left[1 - \exp(-2 \, a \, t)\right] \\ + \frac{b}{a} \left[\langle n_i \rangle(0) + \langle n_j \rangle(0) - \frac{2 \, b}{a} \right] \, \left[\exp(-a \, t) - \exp(-2 \, a \, t)\right], \tag{48}$$

where (27) has been used, and the fact that

$$C_i(t) = \langle n_i \rangle(t). \tag{49}$$

Using (39), one has

$$\dot{F}_{ij} = b_1 C_i + b_2 C_j - (a+1) F_{ij}, \qquad j-i=1,$$
(50)

the solution to which is

$$F_{ij}(t) = \langle n_i n_j \rangle(0) \exp[-(a+1)t] + \frac{b^2}{a(a+1)} \{1 - \exp[-(a+1)t]\} + \left[b_1 \langle n_i \rangle(0) + b_2 \langle n_j \rangle(0) - \frac{b^2}{a}\right] \times \{\exp(-at) - \exp[-(a+1)t]\}, \quad j-i=1.$$
(51)

One thus arrives for an expression for the two point functions:

$$\langle n_{i} n_{j} \rangle(t) = \begin{cases} C_{ij}(t), & j-i > 1\\ F_{ij}(t), & j-i = 1\\ \langle n_{i} \rangle(t), & j-i = 0 \end{cases}$$
(52)

6 Uncorrelated full intervals

A special case of the initial conditions is when

$$D_{\boldsymbol{\ell}}(0) = \prod_{j=0}^{k} \left\langle \prod_{m=1}^{\ell_{2j}} n_{\ell_0 + \dots + \ell_{2j-1} + m} \right\rangle(0), \qquad \forall \, \boldsymbol{\ell}, \tag{53}$$

where

which can be written as

$$D_{\ell}(0) = \prod_{j=0}^{k} F_{\ell_{2j}}(0), \quad \forall \, \ell.$$
(54)

Using (13), it is seen that the ansatz

$$D_{\ell}(t) = \prod_{j=0}^{k} F_{\ell_{2j}}(t),$$
(55)

does satisfy (46). This does not mean that the system is completely uncorrelated, as the ansatz

$$F_n(t) = (F_1)^n(t), (56)$$

does not satisfy (13). But it means that the full intervals are uncorrelated to each other. Among other things, it does mean that the correlators C satisfy

$$C_{i_0\cdots i_k} = (F_1)^{k+1}, (57)$$

if this holds initially.

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