Models solvable through the empty-interval method

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Received 1st May 2005 / Received in final form 22 June 2005 Published online 17 November 2005 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2005

Abstract. The most general one dimensional reaction-diffusion model with nearest-neighbor interactions solvable through the empty interval method, and without any restriction on the particle-generation from two adjacent empty sites is studied. It is shown that turning on the reactions which generate particles from two adjacent empty sites, results in a gap in the spectrum of the evolution operator (or equivalently a finite relaxation time).

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 02.50.Ga Markov processes

1 Introduction

Reaction-diffusion systems have been studied using various methods, including analytical techniques, approximation methods and simulation. The proper approximation methods are generally different in different dimensions, as for example the mean field techniques, working good for high dimensions, generally do not give correct results for low dimensional systems. A large fraction of analytical studies, belong to low-dimensional (specially one-dimensional) systems, where solving low-dimensional systems should in principle be easier [1–13].

In this context, the term solvability (or integrability) is used in different senses. In [14–16], integrability means that the N-particle conditional probabilities' S-matrix is factorized into a product of 2-particle S-matrices. In [17–27], solvability means closedness of the evolution equation of the empty intervals (or their generalization). In [28–30], solvability means that the evolution equation of *n*-point functions contains only *n*- or less- point functions.

Among the important aspects of reaction-diffusion systems, are the stationary state of the system (or one of the quantities describing the system) and the relaxation behavior of the system towards this configuration. In the thermodynamic limit (when the size of the system tends to infinity) these behaviors may show discontinuity in terms of the control parameters of the system. In [31–34] (for example), such behaviors are studied.

The empty interval method (EIM) has been used to analyze the one dimensional dynamics of diffusion-limited coalescence [17–20]. Using this method, the probability that n consecutive sites are empty has been calculated. This method has been used to study a reactiondiffusion process with three-site interactions [22]. EIM has been also generalized to study the kinetics of the q-state one-dimensional Potts model in the zero-temperature limit [21].

In this article, we are going to study all the one dimensional reaction-diffusion models with nearest neighbor interactions which can be exactly solved by EIM. It is worth noting that ben-Avraham et al. have studied one-dimensional diffusion-limited processes through EIM [17–20]. In their study, some of the reaction rates have been taken infinite, and they have worked out the models on continuum. For the cases of finite reactionrates, some approximate solutions have been obtained.

We study models with finite reaction rates, obtain conditions for the system to be solvable via EIM, and then solve the equations of EIM. In [23], general conditions were obtained for a single-species reaction-diffusion system with nearest neighbor interactions, to be solvable through the empty-interval method. Solvability means that evolution equation for E_n (the probability that n consecutive sites be empty) is closed. It turned out there, that certain relations between the reaction rates are needed, so that the system is solvable via EIM. The evolution equation of E_n is a recursive equation in terms of n, and that this equation is linear. 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, which makes them be solved more easily. The criteria for solvability, and the solution of the empty-interval equation were generalized to cases of multispecies systems and multi-site interactions in [24, 26, 27].

Here we want to study the case dropped from the study in [23], namely when there are interactions producing particles from two adjacent empty sites. Doing so, we are considering the most general one dimensional

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reaction-diffusion model with nearest-neighbor interactions which can be solved exactly through EIM.

The scheme of the paper is as follows. In Section 2, the most general one dimensional reaction-diffusion model with nearest-neighbor interactions which can be solved exactly through EIM is introduced. In the same section the evolution equation of the empty intervals is obtained for a lattice. Then, using a limiting procedure a similar equation is obtained for the continuum. In Section 3 the stationary solution to this equation is obtained. In Section 4 the relaxation of the system towards its stationary state is investigated. Section 5 is devoted to the concluding remarks.

2 Models solvable through the empty interval method

To introduce the notation, let us briefly review the criteria that a single-species nearest-neighbor-interaction reaction-diffusion system be solvable through the emptyinterval method (EIM). Consider a one-dimensional lattice. It was shown in [23], that the most general interactions for a single-species model in a one-dimensional lattice with nearest-neighbor interactions are

$$\bullet \circ \to \begin{cases} \bullet \bullet, & r_1 \\ \circ \bullet, & r_2 \end{cases}, \quad \circ \bullet \to \begin{cases} \bullet \circ, & r_3 \\ \bullet \bullet, & r_4 \end{cases}, \quad \bullet \bullet \to \begin{cases} \bullet \circ, & r_3 \\ \circ \bullet, & r_2 \end{cases},$$
(1)

and

$$\circ \circ \to \text{anything}, \qquad r,$$
 (2)

in order that the system be solvable through the EIM. Here an empty (occupied) site is denoted by \circ (•), and r_i 's and r are reaction rates. Denoting the probability of finding n consecutive empty sites by

$$P(\underbrace{\circ \circ \cdots \circ}^{n}) =: E_n, \tag{3}$$

it was then shown that

$$\frac{\mathrm{d}E_n(t)}{\mathrm{d}t} = (r_2 + r_3)(E_{n-1} + E_{n+1} - 2E_n) - (r_1 + r_4)(E_n - E_{n+1}) - (n-1)r E_n, \quad n > 1, \quad (4)$$

$$\frac{\mathrm{d}E_1(t)}{\mathrm{d}t} = (r_2 + r_3)(1 + E_2 - 2E_1) - (r_1 + r_4)(E_1 - E_2),$$
(5)

$$\frac{\mathrm{d}E_{L+1}(t)}{\mathrm{d}t} = -L\,r\,E_{L+1},\tag{6}$$

where the length of the lattice has been assumed to be L+1. It is seen that the equation (5) takes a form similar to equation (4), provided one defines

$$E_0(t) := 1.$$
 (7)

In [23], equations (4) to (6) were actually obtained for the case r = 0. Equations (4) to (7), and of course the initial

values of E_n 's, are a complete set of equations to obtain $E_n(t)$. One can absorb the rate $(r_2 + r_3)$ in the definition of time, and rewrite equations (4) and (5) as

$$\frac{\mathrm{d}E_n(t)}{\mathrm{d}t} = (E_{n-1} + E_{n+1} - 2E_n) - b(E_n - E_{n+1}) - (n-1)cE_n, \qquad 0 < n < L+1, \quad (8)$$

where

$$b := \frac{r_1 + r_4}{r_2 + r_3},$$

$$c := \frac{r}{r_2 + r_3}.$$
 (9)

The aim is to solve equation (8) along with equations (6) and (7).

The continuous-space form of the above equations is

$$\frac{\partial E}{\partial t} = \frac{\partial^2 E}{\partial x^2} + b \frac{\partial E}{\partial x} - c x E, \qquad 0 < x < X, \qquad (10)$$

with the boundary conditions

$$E(x = 0, t) = 1, (11)$$

$$\frac{\partial E(x=X,t)}{\partial t} = -c X E(x=X,t).$$
(12)

The procedure to write these equations in continuous space is to define

$$\begin{aligned} x &:= n \,\Delta, \\ \tilde{t} &:= \Delta^2 t, \\ \tilde{b} &:= \frac{b}{\Delta}, \\ \tilde{c} &:= \frac{c}{\Delta^3}, \\ E(x, \tilde{t}) &:= E_n(t). \end{aligned}$$
(13)

One then expands the right-hand sides of equations (7) and (8) in terms of Δ , sends Δ to zero, and substitutes the quantities with tilde with the corresponding quantities without tilde.

Using the new variable \mathcal{E} defined through

$$\mathcal{E}(x,t) := E(x,t) \, \exp\left(\frac{b\,x}{2}\right),\tag{14}$$

one can rewrite equations (10) to (12) as

$$\frac{\partial \mathcal{E}}{\partial t} = \frac{\partial^2 \mathcal{E}}{\partial x^2} - \left(\frac{b^2}{4} + c x\right) \mathcal{E}, \qquad 0 < x < X, \qquad (15)$$

$$\mathcal{E}(x=0,t) = 1,\tag{16}$$

$$\frac{\partial \mathcal{E}(x=X,t)}{\partial t} = -c \, X \, \mathcal{E}(x=X,t). \tag{17}$$

3 The stationary solution

Denote the stationary solution to equations (10) and (12) by E^{P} . It is seen that \mathcal{E}^{P} is a linear combination of the Airy functions, so,

$$E^{\mathrm{P}}(x) = \exp\left(-\frac{b\,x}{2}\right) \left\{ \alpha \operatorname{Ai}\left[c^{-2/3}\left(c\,x + \frac{b^2}{4}\right)\right] +\beta \operatorname{Bi}\left[c^{-2/3}\left(c\,x + \frac{b^2}{4}\right)\right] \right\}, \quad (18)$$

where α and β are two constants satisfying

$$\alpha \operatorname{Ai}\left(\frac{c^{-2/3}b^2}{4}\right) + \beta \operatorname{Bi}\left(\frac{c^{-2/3}b^2}{4}\right) = 1,$$

$$\alpha \operatorname{Ai} \left[c^{-2/3} \left(c X + \frac{b^2}{4} \right) \right] + \beta \operatorname{Bi} \left[c^{-2/3} \left(c X + \frac{b^2}{4} \right) \right] = 0.$$
(19)

This solution is simplified for $X \to \infty$ (the thermodynamic limit). As $\operatorname{Bi}(y)$ behaves like the exponential of a $y^{3/2}$ for $y \to \infty$, it is seen that in the thermodynamic limit β is zero. So,

$$E^{\mathrm{P}}(x) = \frac{1}{\mathrm{Ai}\left(\frac{c^{-2/3}b^2}{4}\right)} \exp\left(-\frac{bx}{2}\right)$$
$$\times \mathrm{Ai}\left[c^{-2/3}\left(cx + \frac{b^2}{4}\right)\right], \qquad X \to \infty.$$
(20)

It is seen that there is a unique stationary solution.

The above argument is valid for $c \neq 0$. If c = 0, then E(x = X, t), and hence $\mathcal{E}(x = X, t)$, is *t*-independent, and one has

$$E^{\mathrm{P}}(x) = \gamma + (1 - \gamma) \exp(-bx), \qquad c = 0,$$
 (21)

where γ is an arbitrary constant between zero and one. It is seen that in this case the stationary solution is not unique. It is also noteworthy that equation (21) is *not* the limit of equations (18) or (20) as c tends to zero.

4 Relaxation towards the stationary solution

Defining

$$F(x,t) := E(x,t) - E^{P}(x), \qquad (22)$$

it is seen that the evolution equation for F is the same as that of E, except for the fact that the boundary conditions for F are homogeneous. To calculate F(x, t), one seeks the eigenvalues and eigenvectors of the evolution operator:

$$\epsilon f_{\epsilon}(x) = \frac{\mathrm{d}^2 f_{\epsilon}}{\mathrm{d}x^2} + b \frac{\mathrm{d}f_{\epsilon}}{\mathrm{d}x} - c \, x \, f_{\epsilon}, \qquad 0 < x < X, \quad (23)$$

$$f_{\epsilon}(0) = 0, \tag{24}$$

$$\epsilon f_{\epsilon}(X) = -c X f_{\epsilon}(X). \tag{25}$$

The solution to this is

$$f_{\epsilon}(x) = \exp\left(-\frac{b\,x}{2}\right) \\ \times \left\{ \alpha \operatorname{Ai}\left[c^{-2/3}\left(c\,x + \epsilon + \frac{b^2}{4}\right)\right] \\ + \beta \operatorname{Bi}\left[c^{-2/3}\left(c\,x + \epsilon + \frac{b^2}{4}\right)\right] \right\}, \quad (26)$$

where α and β are two constants satisfying

$$\alpha \operatorname{Ai} \left[c^{-2/3} \left(\epsilon + \frac{b^2}{4} \right) \right] + \beta \operatorname{Bi} \left[c^{-2/3} \left(\epsilon + \frac{b^2}{4} \right) \right] = 0,$$

$$\alpha \operatorname{Ai} \left[c^{-2/3} \left(c X + \epsilon + \frac{b^2}{4} \right) \right]$$

$$+ \beta \operatorname{Bi} \left[c^{-2/3} \left(c X + \epsilon + \frac{b^2}{4} \right) \right] = 0. \quad (27)$$

It is seen that the above equations for α and β have nonzero solutions, only for certain discrete values of ϵ . This means that the spectrum of the evolution operator is discrete, and there is a gap between zero and the largest nonzero eigenvalue of the evolution operator. Here too, the solution is simplified if one considers the thermodynamic limit. In this case,

$$f_{\epsilon}(x) = \exp\left(-\frac{b\,x}{2}\right) \operatorname{Ai}\left[c^{-2/3}\left(c\,x + \epsilon + \frac{b^2}{4}\right)\right], \ X \to \infty,$$
(28)

where ϵ is among ϵ_n 's:

$$\epsilon_n := c^{2/3} z_n - \frac{b^2}{4}, \tag{29}$$

and z_n 's are the zeros of the Airy function:

$$\operatorname{Ai}(z_n) = 0. \tag{30}$$

It is seen that if one tends c to zero and X to infinity, the spectrum of the evolution operator tends to $(-\infty, -b^2/4)$. However, if one puts c = 0 and $X = \infty$, and then solves the eigenvector equation, another result is obtained. In this case, equations (23) to (25) become

$$\epsilon f_{\epsilon}(x) = \frac{\mathrm{d}^2 f_{\epsilon}}{\mathrm{d}x^2} + b \frac{\mathrm{d}f_{\epsilon}}{\mathrm{d}x}, \qquad 0 < x, \qquad (31)$$

$$f_{\epsilon}(0) = 0, \tag{32}$$

$$\lim_{x \to \infty} f_{\epsilon}(x) = 0. \tag{33}$$

The solution to these is

$$f_{\epsilon}(x) = \sinh\left(\sqrt{\epsilon + \frac{b^2}{4}}x\right) \exp\left(-\frac{bx}{2}\right),$$
 (34)

and the only condition for ϵ is that ϵ must be negative. That is, the spectrum of the evolution operator is $(-\infty, 0)$.

5 Concluding remarks

The most general one-dimensional single-species exclusion model was considered, for which the evolution of the empty-intervals is closed. The effect of particle creation in two empty adjacent sites was specially investigated. The stationary solution was obtained and the relaxation towards this stationary solution was studied. It was shown that if the rate of particle creation in adjacent empty sites is nonzero, then the spectrum of the evolution operator of the empty intervals is discrete. If this rate is zero and the system is infinite, then the spectrum is continuous. However, the spectrum depends on whether one finds the spectrum for the finite system and then tends the size of the system to infinity, or the spectrum is directly calculated for the infinite system. In the former case, the largest eigenvalue of the evolution operator is negative (there is a gap in the spectrum) and the results of [23] are recovered. This means the the relaxation of the system towards its steady state is exponential, in other words, the system has a finite relaxation time. In the latter case, there is no gap in the spectrum and the spectrum extends to zero. So in this case the relaxation of the system towards its steady state is not exponential, in other words, the relaxation time of the system is infinite. This is an example of a system for which the limit of the spectrum as the size of the system tends to infinity is different from the spectrum of the infinite system [1].

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