Exclusion processes and boundary conditions

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Abstract

A family of boundary conditions corresponding to exclusion processes is introduced. This family is a generalization of the boundary conditions corresponding to the simple exclusion process, the drop-push model, and the one-parameter solvable family of pushing processes with certain rates on the continuum [1–3]. The conditional probabilities are calculated using the Bethe ansatz, and it is shown that at large times they behave like the corresponding conditional probabilities of the family of diffusion-pushing processes introduced in [1–3].

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1 Introduction

In recent years, the asymmetric exclusion process and the problems related to it, including for example the bipolimerization [4], dynamical models of interface growth [5], traffic models [6], the noisy Burgers equation [7], and the study of shocks [8, 9], have been extensively studied. The dynamical properties of this model have been studied in [9, 11]. As the results obtained by approaches like mean field are not reliable in one dimension, it is useful to introduce solvable models and analytic methods to extract exact physical results. Among these methods is the coordinate Bethe-ansatz, which was used in [12] to solve the asymmetric simple exclusion process on a one-dimensional lattice. In [1], a similar technique was used to solve the drop-push model [13], and a generalized one-parameter model interpolating between the asymmetric simple exclusion model and the drop-push model. In [2], this family was further generalized to a family of processes with arbitrary left- and right- diffusion rates. All of these models were lattice models. Finally, the behaviour of latter model on continuum was investigated in [3]. The continuum models of this kind are also investigated in [14, 15]. In [16], another generalization of boundary conditions corresponding to these processes was introduced, which shows an exclusion process with annihilation as well as diffusion. In [17], the Bethe-ansatz method was used to investigate reaction-diffusion processes involving particles of more than one type, on a lattice.

In the generalized model interpolating between the asymmetric simple exclusion model and the drop-push model [1–3], there are two parameters $\lambda$ and $\mu$, which control the pushing rate. Normalizing the diffusion rate to one, it is seen that the sum of these two parameters should be one to ensure the conservation of probability. These two parameters appear in the boundary condition used instead of the reaction. The question is that on continuum, what other kind of boundary conditions, corresponding to other reactions, can be imposed. This is what is investigated in the present paper.

The scheme of the paper is the following. In section 2, the allowed boundary conditions are investigated. The criterion to choose a boundary condition is the conservation of probability. It is shown that the boundary condition is characterized by a one-variable function which vanishes at the origin.

In section 3, the Bethe-ansatz solution for the 2-particle probability of this process is obtained, and its large-time behavior is investigated. It is shown that the large-time behavior of the system is determined by only the first nonzero derivative of the function determining the boundary condition, at the origin. If this function does have a nonvanishing linear term, then that term determines the large-time behavior of the system, and the results of [3] are recovered.

Finally, in section 4, boundary conditions are investigated for which the first derivative of the function determining the boundary condition vanishes at the origin. The mean position of the particles, and the effective diffusion parameter are obtained.
2 Boundary conditions

Consider a collection of \( N \) particles diffusing on a one-dimensional continuum. So long as the particles do not encounter each other, the master equation governing the probability density of finding these at \( x_1 < \cdots < x_N \) is [3]

\[
\frac{\partial}{\partial t} P(x; t) = \frac{1}{2} \nabla^2 P(x; t). \tag{1}
\]

In [3], it was shown that the exclusion pushing condition can be written as a boundary condition with two parameters (in fact with only one independent parameter, since \( \lambda + \mu = 1 \)):

\[
\left( \mu \frac{\partial}{\partial x_i} P - \lambda \frac{\partial}{\partial x_{i+1}} \right) P \bigg|_{x_{i+1}=x_i} = 0. \tag{2}
\]

To obtain this system, in [3] it was started with a collection of particles diffusing on a one-dimensional lattice. Each particle diffuses to the right with the rate one, if the right site is free. If the right site is occupied, the particle may push other particles and go to the right, with a special rate. That is, we have the following process.

\[
\underbrace{AA\cdots A}_{n} \emptyset \rightarrow \emptyset \underbrace{AA\cdots A}_{n}, \quad \text{with the rate } r_n, \tag{3}
\]

where

\[
r_n := \left[ 1 + \cdots + \left( \frac{\lambda}{\mu} \right)^n \right]^{-1}. \tag{4}
\]

It was shown in [1], that such a system can be described by the master equation

\[
\dot{P}(x; t) = \sum_i P(x - \mathbf{e}_i; t) - N P(x; t), \quad x_1 < \cdots < x_N, \tag{5}
\]

subject to the boundary condition

\[
P(\ldots, x_i = x, x_{i+1} = x, \ldots; t) = \lambda P(\ldots, x_i = x, x_{i+1} = x+1, \ldots; t) + \mu P(\ldots, x_i = x-1, x_{i+1} = x, \ldots; t). \tag{6}
\]

In [5], \( \mathbf{e}_i \) is a vector the components of which are all zero, except for the \( i \)'th component, which is one. In [3], (1) and (2) were obtained as the limit of (5) and (6) when the probability is a slowly-varying function, with a suitable Galileo transformation, so that one has diffusion to right and left (with equal rates). So, (1) and (2) describe a system of particles diffusing on a continuum and pushing each other with certain rates, as introduced in (3) and (4).

For the special case \( N = 2 \), (1) and (2) become

\[
\frac{\partial}{\partial t} P(x_1, x_2; t) = \frac{1}{2} (\partial_1^2 + \partial_2^2) P(x_1, x_2; t), \tag{7}
\]
and
\[ \mu \partial_1 P(x, x) = \lambda \partial_2 P(x, x). \] (8)

Using
\[ \partial P(x, x) = \partial_1 P(x, x) + \partial_2 P(x, x), \] (9)

it is seen that the boundary condition (8) is equivalent to
\[ (\partial_1 - \partial_2)P(x, x) = (\lambda - \mu)\partial P(x, x). \] (10)

The passage from (6) to (2) is not unique. But any boundary condition has to ensure probability conservation. Consider the evolution (7), and note that it is valid only for the physical region \( x_1 < x_2 \). Integrating this over the physical region, one arrives at
\[ \frac{d}{dt} \int dx_1 dx_2 P(x_1, x_2) = \frac{1}{2} \int_{-\infty}^{+\infty} dx (\partial_1 - \partial_2)P(x, x). \] (11)

But using (10), it is seen that the right-hand side of (11) is zero. So,
\[ \frac{d}{dt} \int dx_1 dx_2 P(x_1, x_2) = 0. \] (12)

This is the conservation of probability. However, the only thing needed to ensure this conservation is that \((\partial_1 - \partial_2)P(x, x)\) be a total derivative of some function with respect to \( x \). So, one can in general use a boundary condition like
\[ (\partial_1 - \partial_2)P(x, x) = \alpha_1 \partial P(x, x) + \alpha_2 \partial \partial P(x, x) + \cdots = f(\partial)P(x, x), \] (13)

where \( f \) is an analytic function satisfying
\[ f(0) = 0. \] (14)

Such a boundary condition ensures probability conservation. In [16], a slightly different boundary condition was introduced, which in this language is equivalent to \( f(0) < 0 \). It was seen there such a boundary condition describes annihilation as well as diffusion.

3 The Bethe-ansatz solution

The Bethe-ansatz solution to the Master equation (11), with the boundary condition (13) is
\[ P(x; t) = e^{Et\Psi(x)}, \] (15)

where \( \Psi \) satisfies
\[ E\Psi(x) = \frac{1}{2} \nabla^2 \Psi(x), \] (16)
and the boundary condition (13). The solution to these, is

$$\Psi_k(x) = \sum_\sigma A_\sigma e^{i\sigma(k) \cdot x},$$  
(17)

with

$$E = -\frac{1}{2} \sum_i k_i^2,$$  
(18)

provided one can find $A_\sigma$’s so that (13) is satisfied. The summation in (17) is over the permutations of $N$ objects, Applying (13) to the case $x_j = x_{j+1}$, one obtains

$$i [k_{\sigma(j)} - k_{\sigma(j+1)}] (A_\sigma - A_{\sigma\sigma_j}) = i [\tilde{f}(k_{\sigma(j)}) + \tilde{f}(k_{\sigma(j+1)})] (A_\sigma + A_{\sigma\sigma_j}),$$  
(19)

where $\tilde{f}$ is defined as

$$\tilde{f}(k) := - i f(ik),$$  
(20)

and $\sigma_j$ is that permutation which changes $j$ to $j + 1$ and vice versa, and leaves other numbers unchanged. From (19), $A_\sigma$ can be obtained as

$$A_{\sigma\sigma_j} = S(k_{\sigma(j)}, k_{\sigma(j+1)}) A_\sigma,$$  
(21)

where

$$S(k_1, k_2) = \frac{k_2 - k_1 + \tilde{f}(k_1 + k_2)}{k_2 - k_1 - \tilde{f}(k_1 + k_2)}$$

$$= 1 + \frac{2\tilde{f}(k_1 + k_2)}{k_2 - k_1 - \tilde{f}(k_1 + k_2)},$$  
(22)

As $\sigma_1 \sigma_2 \sigma_1 = \sigma_2 \sigma_1 \sigma_2$, the coefficients $A$, should satisfy the consistency condition

$$A_{\sigma_1 \sigma_2 \sigma_1} = A_{\sigma_2 \sigma_1 \sigma_2}.$$  
(23)

The above criterion, in terms of $S$ is

$$S(k_2, k_3) S(k_1, k_3) S(k_1, k_2) = S(k_1, k_2) S(k_1, k_3) S(k_2, k_3),$$  
(24)

which is obviously an identity.

Using this Bethe-ansatz solution, the conditional probability can be written as

$$P(x; t | y; 0) = \int \frac{dk^N}{(2\pi)^N} \Psi_k(x) e^{E(k)t - ik \cdot y},$$  
(25)

where in $\Psi_k$, the coefficient of $e^{ik \cdot x}$ is set to be equal to one.

This shows the integrability of the system, in the sense that the $N$-particle scattering matrix ($A_\sigma$’s) can be expressed as a product of two-particle scattering matrices.
3.1 The conditional probability for the 2-particle sector

The conditional probability for the 2-particle sector, is written as

\[ P(x; t|y; 0) = \frac{1}{4\pi^2} \int dk_1 dk_2 \left[ e^{ik_1 x_1 + ik_2 x_2} + S(k_1, k_2) e^{ik_1 x_2 + ik_2 x_1} \right] e^{Et - ik \cdot y}, \]

so that it satisfies (7) and the initial condition

\[ P(x, 0|y, 0) = \delta(x_1 - y_1)\delta(x_2 - y_2) \]

for the physical region \((x_1 < x_2, \quad y_1 < y_2)\).

Using the form of \(S\), one can write this conditional probability as

\[ P(x; t|y; 0) = \frac{1}{2\pi^2} \left\{ e^{i(k_1 x_1 + k_2 x_2)} \right. \]

\[ + \left[ 1 + \frac{2\tilde{f}(k_1 + k_2)}{k_2 - k_1 - \tilde{f}(k_1 + k_2)} \right] e^{i(k_1 x_2 + k_2 x_1)} \}.
\]

(28)

In the above integration, the possible ambiguity arising from the pole of the fraction is removed through \(k_1 \rightarrow k_1 + i \varepsilon\) and \(k_2 \rightarrow k_2 - i \varepsilon\), where the \(\varepsilon \rightarrow 0^+\) limit of the integral is meant. This ensures that the probability tends to zero as \(x_1 \rightarrow -\infty\) or \(x_2 \rightarrow +\infty\).

The two first integrals of the right-hand side are easily calculated. So,

\[ P(x; t|y; 0) = \frac{1}{2\pi t} \left\{ e^{-[(x_1 - y_1)^2 + (x_2 - y_2)^2]/(2t)} + e^{-(z_1^2 + z_2^2)/2t} \right\} + I_3, \]

where

\[ z_1 := x_1 - y_2, \quad z_2 := x_2 - y_1. \]

(30)

To obtain the third integral \((I_3)\), one uses the change of variable

\[ k := k_1 + k_2, \quad q := k_2 - k_1 - \tilde{f}(k_1 + k_2). \]

(31)

Then,

\[ I_3 = \int \frac{dk dq}{4\pi^2} \frac{\tilde{f}(k)}{q} e^{-t(k^2 + |q + \tilde{f}(k)|^2)/4} e^{i(kA_2 + |q + \tilde{f}(k)|A_1)/2} \]

\[ = \sqrt{\frac{\pi}{t}} \int \frac{dk}{4\pi^2} \tilde{f}(ik) e^{i(kA_2 + A_1 f(ik))/2} e^{-tk^2/4} \]

\[ \times \int_{-\infty}^{A_1} dA e^{-[A^2 + 2At f(ik)]/(4t)}, \]

(32)

where

\[ A_1 := z_1 - z_2, \quad A_2 := z_1 + z_2. \]

(33)
Simplifying (32), one arrives at

\[ I_3 = \sqrt{\frac{\pi}{t}} \int \frac{dk}{4\pi^2} \int_{-\infty}^{A_1} dA f \left( 2 \frac{\partial}{\partial A_2} \right) e^{\frac{A_1 - A}{2}} f \left( 2 \frac{\partial}{\partial A_2} \right) \]

\[ \times e^{-\frac{tk^2}{4} - 2ikA_2} e^{-\frac{A^2}{4t}} \]

\[ = \frac{1}{2\pi^4} \int_{-\infty}^{A_1} dA f \left( 2 \frac{\partial}{\partial A_2} \right) e^{\frac{A_1 - A}{2}} f \left( 2 \frac{\partial}{\partial A_2} \right) e^{-\frac{A^2 + A_2^2}{4t}}. \quad (34) \]

To show that (29) does indeed satisfy the initial conditions, first note that

\[ P(x; 0|y; 0) = \delta(x_1 - y_1) \delta(x_2 - y_2) + \delta(x_1 - y_2) \delta(x_2 - y_1) + I_3(t = 0). \quad (35) \]

The second term is obviously zero in the physical region \( x_1 < x_2 \) and \( y_1 < y_2 \). For the third term, we have from the first equality in (32)

\[ I_3(t = 0) = \int \frac{dk}{4\pi^2} \hat{f}(k) e^{\frac{ikA_2 + A_1 f(k)}{2}} \int \frac{dq}{q - i\varepsilon} e^{iqA_1/2}. \quad (36) \]

The integral over \( q \) is, however, zero in the physical region. Since in the physical region \( A_1 < 0 \), and one can close the integration contour by adding a large semicircle in the lower half plane of \( q \), to the real line. There are no singularities inside the closed contour, so the integral vanishes. So (29) does indeed satisfy the initial conditions.

Now consider the large-time behavior of the system. Using the change of variable

\[ A_i = 2a_i \sqrt{t}, \quad (37) \]

the integral \( I_3 \) becomes

\[ I_3 = \frac{1}{\pi t} \int_{-\infty}^{a_1} da \sqrt{t} f \left( \frac{1}{\sqrt{t} \partial \partial_2} \right) e^{\sqrt{t}(a_1 - a)} f \left( \frac{1}{\sqrt{t} \partial \partial_2} \right) e^{-(a_1^2 + a_2^2)}. \quad (38) \]

It is seen that at large times, the dominant term comes from the first nonzero term in the expansion of \( f \). This means that if the first derivative of \( f \) does not vanish at the origin, then at large times, \( f \) is equivalent to a linear function. But a linear \( f \) is just the boundary condition used in [3]. So at large times, the boundary condition has effectively only one free parameter determining the interaction.

If \( f \) is an at-most-quadratic polynomial, then the integration over \( k \) in (32) can be done. For the simple example

\[ f(x) = \alpha_2 x^2, \quad (39) \]
the result would be

\[
I_3 = \alpha \int_{-\infty}^{\infty} \frac{dA}{2\pi} \left\{ \frac{A^2}{[t + 2\alpha(A - A_1)]^2} - \frac{2}{t + 2\alpha(A - A_1)} \right\}
\times \frac{1}{\sqrt{t[t + 2\alpha(A - A_1)]}} e^{\frac{A^2}{2\alpha} \sin^2(A - \alpha_1)}.
\]  \quad (40)

4 Boundary conditions corresponding to functions \(f\) with vanishing first derivative at the origin

Taking the form

\[
f(x) = \alpha_n x^n + O(x^{n+1})
\]  \quad (41)

for \(f\) (where \(n > 1\)), it is seen from (38) that at large times, the leading term of \(I_3\) is

\[
I_3 \sim \frac{\alpha_n}{\pi \sqrt{t^{n+1}}} \int_{-\infty}^{\infty} da \frac{\partial^n}{\partial a^2} e^{-(a^2 + a_1^2)}.
\]  \quad (42)

The integration in the left-hand side, can now be easily done, and one arrives at

\[
I_3 \sim \frac{\alpha_n}{2 \sqrt{\pi t^{n+1}}} [1 + \text{erf}(a_1)] \frac{\partial^n}{\partial a^2} e^{-a_2^2}.
\]  \quad (43)

Two important quantities to be calculated, are the mean position of the particles, and the variance of the mean position. The expectation value of any function \(g(x_1, x_2)\), is obtained through

\[
\langle g(x_1, x_2) \rangle := \int_{x_1 \leq x_2} d^2x \, P(x|y)g(x_1, x_2),
\]

\[
= \langle g(x_1, x_2) \rangle_0 + \langle g(x_1, x_2) \rangle_3,
\]  \quad (44)

where

\[
\langle g(x_1, x_2) \rangle_3 := \int_{x_1 \leq x_2} d^2x \, I_3(x_1, x_2)g(x_1, x_2),
\]

\[
= 2t \int_{-\infty}^{\infty} da_2 \int_{-\infty}^{(y_1 - y_2)/(2\sqrt{t})} da_1 \, I_3(x_1, x_2)g(x_1, x_2),
\]  \quad (45)

and

\[
\langle g(x_1, x_2) \rangle_0 := \int_{x_1 \leq x_2} d^2x \, \frac{1}{2\pi t} e^{-[(x_1 - y_1)^2 + (x_2 - y_2)^2]/(2t)} g(x_1, x_2),
\]

\[
+ \int_{x_1 \geq x_2} d^2x \, \frac{1}{2\pi t} e^{-[(x_1 - y_1)^2 + (x_2 - y_2)^2]/(2t)} g(x_2, x_1).
\]  \quad (46)
If \( g(x_1, x_2) = g(x_2, x_1) \), then the above expression becomes simpler:

\[
\langle g(x_1, x_2) \rangle_0 = \int d^2x \frac{1}{2\pi t} e^{-[(x_1-y_1)^2+(x_2-y_2)^2]/(2t)} g(x_1, x_2).
\] (47)

Using these, we want to calculate

\[
X := \frac{1}{2}(x_1 + x_2),
\] (48) and

\[
(\Delta X)^2 := \frac{1}{2}(x_1^2 + x_2^2) - X^2.
\] (49)

Using (47), it is easily seen that

\[
X_0 = \frac{y_1 + y_2}{2},
\] (50) and

\[
\frac{1}{2}(x_1^2 + x_2^2)_0 = (X_0)^2 + t.
\] (51)

From (38), it is seen that \( I_3 \) is the \( n \)'th derivative of some function with respect to \( a_2 \). So, if \( g \) is a polynomial of order less than \( n \) with respect to \( a_2 \), the right-hand side of (44) vanishes; this can be seen through \( n \) times integration by parts. The functions relevant to the calculation of the mean position and the variance, in terms of \( a_1 \) and \( a_2 \), are polynomials of \( a_1 \) and \( a_2 \) of at most the second degree. From (44), it is seen then that only \( \langle a_2^2 \rangle_3 \) may be nonvanishing, and that even this term vanishes if \( n > 2 \). So, for \( n > 2 \) we have \( X = X_0 \) and \( \text{Var} = \text{Var}_0 \). For \( n = 2 \), it is seen that \( I_3 \) contains second and higher derivatives of functions with respect to \( a_2 \). In calculating \( \langle a_2^2 \rangle_3 \), only the second derivatives are relevant. That is, one can write

\[
I_3 = \frac{\alpha_2}{2\sqrt{\pi t}} [1 + \text{erf}(a_1)] \frac{\partial^2}{\partial a_2^2} e^{-a_2^2} + \bar{I}_3,
\] (52)

where \( \bar{I}_3 \) is irrelevant to the calculation of \( \langle a_2^2 \rangle_3 \). So, one arrives at

\[
\langle a_2^2 \rangle_3 = \frac{2\alpha_2}{\sqrt{\pi}} \int_{-\infty}^{(y_1-y_2)/(2\sqrt{t})} da_1 [1 + \text{erf}(a_1)].
\] (53)

Using

\[
x_1^2 + x_2^2 = \frac{1}{2}(A_1^2 + A_2^2) + B,
\] (54)

where \( B \) is a first order polynomial, one arrives at

\[
\frac{1}{2}(x_1^2 + x_2^2)_3 = t \langle a_2^2 \rangle_3
\]

\[
= 2\alpha_2 \sqrt{t} \int_{-\infty}^{(y_1-y_2)/(2\sqrt{t})} da_1.
\] (55)
From this, (51), and the fact the mean does not depend on $f$ (so long as the first derivative of $f$ vanishes at the origin) it is seen that

$$\text{Var} = t + 2\alpha_2 \sqrt{t} \int_{-\infty}^{(y_1-y_2)/(2\sqrt{t})} da_1 [1 + \text{erf}(a_1)].$$

(56)

This becomes even simpler at large times. At large times, the upper limit in the above integral tends to zero. So, using

$$\int_{-\infty}^{0} [1 + \text{erf}(x)]dx = \frac{1}{\sqrt{\pi}},$$

(57)

one arrives at

$$\text{Var} = t + 2\alpha_2 \sqrt{t/\pi} + O(t^{-1/2}).$$

(58)

The effective diffusion parameter is defined as the derivative of the above:

$$\frac{d\text{Var}}{dt} = 1 + \frac{\alpha_2}{\sqrt{\pi t}} + O(t^{-3/2}).$$

(59)

It is seen that as $t \to \infty$, this parameter tends to one, in agreement with [3,12].
References

[1] M. Alimohammadi, V. Karimipour, & M. Khorrami; Phys. Rev. E57 (1998) 6370.
[2] M. Alimohammadi, V. Karimipour, & M. Khorrami; J. Stat. Phys. 97 (1999) 373.
[3] F. Roshani & M. Khorrami; Phys. Rev. E60 (1999) 3393.
[4] C. T. MacDonald, J. H. Gibbs, & A. C. Pipkin; Biopolymers 6 (1968) 1.
[5] J. Krug & H. Spohn; in Solids far from equilibrium, edited by C. Godreche (Cambridge University Press, Cambridge, England, 1991), and references therein.
[6] K. Nagel; Phys. Rev. E53 (1996) 4655.
[7] J. M. Burgers, The nonlinear diffusion equation (Reidel, Boston, 1974).
[8] B. Derrida, S. A. Janowsky, J. L. Lebowitz, & E. R. Speer; Europhys. Lett. 22 (1993) 651.
[9] P. A. Ferrari & L. R. G. Fontes; Probab. Theory Relat. Fields 99 (1994) 305.
[10] T. Ligget, Interacting particle systems (Springer Verlag, New York, 1985).
[11] L. H. Gava & H. Spohn; Phys. Rev. A46 (1992) 844.
[12] G. M. Schütz; J. Stat. Phys. 88 (1997) 427.
[13] G. M. Schütz & E. Domany; J. Stat. Phys. 72 (1993) 277.
[14] T. Sasamoto & M. Wadati; J. Phys. Soc. Japan 67 (1998) 784.
[15] T. Sasamoto & M. Wadati; J. Phys. A31 (1998) 6057.
[16] F. Roshani & M. Khorrami; J. Math. Phys. 43 (2002) 2627.
[17] F. Roshani & M. Khorrami; Phys. Rev. E64 (2001) 011101.