Integrable Boundary Conditions in Asymmetric Diffusion Processes

Akira Fujii

Universität zu Köln, Institut für Theoretische Physik, 50937 Köln, Germany

Abstract

We study the asymptotic diffusion processes with (generally nonlocal) open boundaries in one dimension which are exactly solvable by means of the recently developed recursion formula. We investigate the stationary states, which cannot be determined in an elementary way. We give the equation which includes an auxiliary parameter and determines possible boundary conditions for the model to be solved exactly. With the help of that equation, we analyze the density current and concentration. We classify the phases according to them.

1 Introduction

The study of the systems with reaction and diffusion in one dimension has been an attracting problem. For example, models including both reaction and diffusion have been considered in view of chemical processes like $A + B \rightarrow C + D$, where $A,B,C$ and $D$ represent some sorts of molecules. Models with only pure diffusion are not trivial, either. They have been studied in relation with interface growth, traffic flow and so on. Some experiments corresponding with the recent theoretical developments have been proceeded. Recently, a problem concerning protein synthesis has been considered in this scheme. To investigate reaction-diffusion models, a variety of methods have been used. Once taking a continuum limit, traditional technique of the field theory such as renormalization group method, mean-field or variational approximation are available.

In this paper, we consider the models on a one-dimensional discretized lattice. Some of the models on a lattice are shown to be integrable by means of the Jordan-Wigner transformation, Bethe ansatz and so on.

The definitions and notations of reaction-diffusion models considered in this paper are as follows. We consider a one-dimensional lattice, where lattice sites are numbered $1, 2, \cdots, L (= \text{the number of sites})$, and several sorts of particles living on the lattice. The total number of particles is not larger than that of lattice sites, i.e. empty sites represented by $\phi$ are allowed. The stochastic process obeys the following continuous flow chart.

1. At an instant $t$, a pair of neighboring sites, say the $i$-th and $(i+1)$-th sites, is chosen randomly.

   We assume that the sorts of particles on the $i$-th and $(i+1)$-th sites are $A$ and $B$, respectively.

2. The particles on $i$ and $i+1$ (A and B) react into the same or other sorts of particles C and D respectively in an infinitesimal time interval $dt$ with a given probability $w_{C\rightarrow A, D\rightarrow B}(C, D)dt$. This process is represented by $A + B \rightarrow C + D$ and we must tell the difference of the order of particles (or sites), i.e. $A + B$ is different from $B + A$ in general.

3. The time should be set $t \rightarrow t + dt$.

4. A process is repeated until $t$ amounts to the final time $t_f$ defined properly. We often put $t_f = +\infty$.

1 e-mail: af@thp.uni-koeln.de
In this paper, we concentrate in models including only particles of one species, $A$, and the parameters $\mu, \nu, \alpha$ and $\beta$ in $w^i_{\alpha,\beta}(\mu, \nu)$ being $\mathbb{Z}_2$ variables. Because of the preservation of the probability, we have the relation

$$w^i_{0,0}(\mu, \nu) = \sum_{r,s} w^i_{r,s}(\mu - r, \nu - s),$$  \hspace{1cm} (1)

hereafter $\sum'$ means that $n_1 = n_2 = \cdots = 0$ in the summation is excluded. Let us introduce the probability distribution $P_L(\tau_1, \cdots, \tau_L; t)$ meaning the probability to find the $i$-th site to be occupied by $A$ (empty) if $\tau_i = 1$ ($0$) at the time $t$. The time evolution equation of $P_L$ is a linear one denoted as

$$\frac{\partial}{\partial t}P_L(\tau_1, \cdots, \tau_L; t) = (\hat{H}P_L)(\tau_1, \cdots, \tau_L; t),$$  \hspace{1cm} (2)

where $\hat{H}$ is a linear operator called Hamiltonian on the analogy of the Schrödinger equation. Needless to say, $H$ can be written in terms of the local interactions characterized by $w$'s as we will see later. We consider the ground state, a solution of $\hat{H}P_L = 0$, which the system will reach after a long time.

Especially, we deal with the problems of the stationary state of an open chain with pure asymmetric exclusion processes (ASEP). Although the setting is quite simple, to obtain the exact form of the stationary state is not easy. With some classes of models, useful recursion relations to determine physical quantities were indicated by Derrida, Domany and Mukamel (DDM) [9]. They solved the recursion relation for a special case and predicted the phase diagram by means of the mean-field approximation. The solutions with general local boundary condition were obtained by Schütz and Domany (SD) without using the mean-field approximation [10].

In this paper, we will consider general boundary conditions including nonlocal boundary interactions so that a recursion relation similar to DDM’s might be available, i.e. integrable. We calculate some physical quantities, the partition function, density current and concentration (one-point function), exactly and classify the phases of the system. The plan of this paper is as follows. In the following $\S 2$, we have a brief sketch of the previous works by DDM and SD. An equation for the possible integrable boundary conditions is given in $\S 3$. We calculate the partition function, density current and concentration in $\S 4$ and $\S 5$. An unknown example is analyzed in $\S 6$. Section $\S 7$ is left for the summary and conclusion.

2 Asymmetric Exclusion Process

In this section, we consider pure-diffusion systems with boundaries, i.e. open chains. Although it seems to be very simple, even determination of the ground state is not easy. An epoch-making work in this field was done by DDM [9]. They made use of a recursion relation among the ground state with different lattice length, and obtained the solution for a special case ($\alpha = \beta = 1$ in the later notation). The phase diagram classified by the strengths of the boundary injection and subtraction rates were conjectured by means of the mean-field approximation. SD proved DDM’s conjecture to be true by obtaining the exact form of the solutions for the general boundary conditions. Another remarkable succeed is development of the so-called matrix product method introduced in ref. [11]. This method enables correlation functions to be calculated algebraically and exactly. Several extension can be found in refs. [12, 13, 14, 15, 16], for example. Recently, this method has been applied for the models including coagulation and decoagulation as well as pure diffusion [17].

In this section, we concentrate in the simplest ASEP model on a lattice with length $L$ [9] defined as follows.
1. Left edge \((i = 1)\)
   At the left edge, the injection and extraction of a particle are possible
   \[ \Phi \rightarrow A \quad \text{with a rate} \quad w_1(1) = \alpha \]
   or
   \[ A \rightarrow \Phi \quad \text{with} \quad w_1(0) = \gamma. \]

2. Bulk property \((i = 1, \cdots, L)\)
   Only diffusion is allowed in the bulk like
   \[ A + \Phi \rightarrow \Phi + A \quad \text{with} \quad w_{11}(01) = p \]
   or
   \[ \Phi + A \rightarrow A + \Phi \quad \text{with} \quad w_{11}(10) = q. \]

3. Right edge \((i = L)\)
   At the right edge, the injection and extraction of a particle are possible as well as at the left edge.
   \[ \Phi \rightarrow A \quad \text{with} \quad w'_1(1) = \delta \]
   or
   \[ A \rightarrow \Phi \quad \text{with} \quad w'_1(0) = \beta. \]

We assume the conservation of the probability, for example
\[ \Phi \rightarrow \Phi \quad \text{with} \quad 1 - \alpha \]
at the left edge. The Hamiltonian of this model can be shown to be equivalent to that of \(XXZ\) spin chain with integrable boundary terms[13, 18]. In this section, we consider the case with \(q = \gamma = \delta = 0\) for simplicity. Considering the rescaling of the time, we can put \(p = 1\) without any loss of the generality. We are interested in the stationary solution of the equation

\[
0 = \sum_{\sigma_1 = 0,1} (h_1)_{\tau_1}^{\sigma_1} P_L(\sigma_1, \tau_2, \cdots, \tau_L) \\
+ \sum_{i=1}^{L-1} \sum_{\sigma_i, \sigma_{i+1} = 0,1} h_{\tau_i, \tau_{i+1}}^{\sigma_i \sigma_{i+1}} P_L(\tau_1, \cdots, \tau_{i-1}, \sigma_i, \tau_{i+1}, \sigma_{i+2}, \cdots, \tau_L) \\
+ \sum_{\sigma_L = 0,1} (h')_{\tau_L}^{\sigma_L} P_L(\tau_1, \cdots, \tau_{L-1}, \sigma_L), \tag{3}
\]
where

\[ h_1 = \begin{pmatrix} \alpha & -\gamma \\ -\alpha & \gamma \end{pmatrix} = \begin{pmatrix} \alpha & 0 \\ -\alpha & 0 \end{pmatrix}, \tag{4} \]

\[ h = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & p & -q & 0 \\ 0 & -p & q & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5} \]

\[ h' = \begin{pmatrix} \delta & -\beta \\ -\delta & \beta \end{pmatrix} = \begin{pmatrix} 0 & -\beta \\ 0 & \beta \end{pmatrix}. \tag{6} \]

The readers should remember that we do not have to restrict parameters less than one once we write the master equation in the above form by rescaling the time. We can consider that they are arbitrary positive numbers.

In DDM’s and the following work, it has been found that the solution of eq.(3) with general \( p, q, \alpha, \beta, \gamma \) and \( \delta \) satisfies surprising recursion relations for \( L \) as follows.

\[ \sum_{\sigma_1=0,1} (h_1)_{\tau_1} \sigma_1 P_L(\sigma_1, \tau_2, \cdots, \tau_L) = -x_{\tau_1} P_{L-1}(\tau_2, \cdots, \tau_L), \tag{7} \]

\[ \sum_{i=1}^{L-1} \sum_{\sigma_i, \sigma_{i+1}=0,1} (h_{\tau_i, \tau_{i+1}})_{\tau_{i+1}} \sigma_{i+1} P_L(\tau_1, \cdots, \tau_{i-1}, \sigma_i, \sigma_{i+1}, \tau_{i+2}, \cdots, \tau_L) = x_{\tau_1} P_{L-1}(\tau_1, \cdots, \tau_{i-1}, \tau_{i+1}, \cdots, \tau_L) - x_{\tau_{i+1}} P_{L-1}(\tau_1, \cdots, \tau_i, \tau_{i+2}, \cdots, \tau_L), \tag{8} \]

\[ \sum_{\sigma_L=0,1} (h'_{\tau_L})_{\tau_L} \sigma_L P_L(\tau_1, \cdots, \tau_{L-1}, \cdots, \sigma_L) = x_{\tau_L} P_{L-1}(\tau_1, \cdots, \tau_{L-1}), \tag{9} \]

where \( x_0 \) and \( x_1 \) are some numbers, which can be set as \(-x_0 = x_1 = 1\). It should be remarked that the normalization property of the probability, \( \sum P_L(\sigma_1, \cdots, \sigma_L) = 1 \) is no more correct. We must renormalize the distribution function after obtaining its form\(^9, 10\). We consider the normalization, \( i.e. \) partition function, in \( \textsection 4 \) in detail.

With the help of this recursion, we can calculate the correlation functions, for example the concentration, with arbitrary \( L \) in principle. Contrary to the calculation of the concentration, those of general \( n \)-point function are difficult, in fact. Some technology to calculate the general correlation functions like the matrix product method\(^11\) have been developed.

### 3 General Boundary Condition

As we have seen in the previous section, the recursion relation (7)-(9) will play a crucial role to solve the model exactly. We consider this recursion relation in detail. In general, we consider a system denoted symbolically by

\[ \circ - \circ - \circ - \cdots - \circ - \circ, \quad n = 0, 1, 2, \ldots \]
Here we introduce an $s$-valued variable $X(= P_1, \ldots, P_s)$ living on $\otimes$ at the left edge and a usual 2-valued variable $\sigma(=0,1)$ on $\circ$. Let us denote $X \in V_s$ and $\sigma \in V_2$ from now. The connection $- \circ - \circ -$ represents a pure asymmetric hopping, which we put $p = 1$ and $q = 0$ in this section. At the right edge ($\circ$), a particle is extracted with $\beta = 1$, $\delta = 0$.

Denoting the distribution function for the ground state as $f_n(X, \sigma_0, \ldots, \sigma_n)$, the master equation takes the following form

$$0 = \sum_{Y \in V_s} \sum_{\rho_0} H_{X \sigma_1}^{Y \rho_0} f_n(Y, \rho_0, \sigma_1, \ldots, \sigma_n)$$

$$+ \sum_{i=0}^{n-1} h_{\sigma_i \sigma_{i+1}}^{\rho_i \rho_{i+1}} f_n(X, \sigma_0, \ldots, \sigma_{i-1}, \rho_i, \rho_{i+1}, \sigma_{i+2}, \ldots, \sigma_n) + (h')_{\sigma_n}^{\rho_n} f_n(X, \sigma_0, \ldots, \sigma_{n-1}, \rho_n)$$

(10)

with the boundary matrix $H_{X \sigma}^Y$, which will be determined later. Other matrices $h$ and $h'$ are defined in eqs. (5) and (6) with $p = 1$, $q = 0$, $\beta = 1$ and $\delta = 0$.

For example, let us consider the simplest ASEP model to make the notation clear. In this case, we can set $X \in V_2$ (i.e. $P_1 = 1$, $P_2 = 0$) and

$$H_{\sigma \sigma'}^{\rho \rho'} = h_{\sigma \sigma'}^{\rho \rho'} + (h_1)^{\rho \rho'}$$

It is obvious that we can reformulate the simplest ASEP model with $X \in V_2$. Anyway, that model can be considered as the simplest example in the following formalism. We want to answer the following question.

**Problem:** What is the condition for the recursion relation

$$f_n(X, \rho_0, \rho_1, \ldots, \rho_{n-1}, 1) = f_{n-1}(X, \rho_0, \rho_1, \ldots, \rho_{n-1}) \quad \text{for } n = 1, 2, \ldots$$

(11)

This relation comes from the recursion relation (10). We look for the answer to the above question. To begin with, we write down the master equation (10) explicitly. For $n = 0$, we can easily obtain

$$\sum_{Y \in V_s, \rho = 0,1} H_{X1}^{Y \rho} f_0(Y, \rho) + f_0(X, 1) = 0,$$

(12)

$$\sum_{Y \in V_s, \rho = 0,1} H_{X0}^{Y \rho} f_0(Y, \rho) - f_0(X, 1) = 0,$$

(13)

which corresponds to the initial condition for the distribution function in the following consideration. Next we consider the equation for $n = 1$;

$$\sum_{Y, \sigma_1} H_{X \rho_1}^{Y \sigma_1} f(Y, \sigma_1, \rho_2) + h_{\rho_1 \rho_2}^{\sigma_1} f(X, \sigma_1, \sigma_2) + (h')_{\rho_2}^{\sigma_2} f(X, \rho_1, \sigma_2) = 0.$$

The independent elements of the above equation are the following three,

$$\sum_{Y, \sigma} H_{X1}^{Y \sigma} f_1(Y, \sigma, 0) + f_0(X, 0) = 0,$$

(14)

$$\sum_{Y, \sigma} H_{X0}^{Y \sigma} f_1(Y, \sigma, 0) - f_0(X, 0) = 0,$$

(15)

$$f_1(X, 1, 0) = f_0(X, 1) + f_0(X, 0).$$

(16)
where we made use of the relation (11) and eq.(16) takes the same form as that for the simplest ASEP model. Similarly, for general \( n(>0) \), we obtain the equation
\[
\sum_{Y,\sigma} H_{X1}^Y f_n(Y,\sigma,0,0,\ldots,0) + f_{n-1}(X,0,\ldots,0) = 0, \tag{17}
\]
\[
\sum_{Y,\sigma} H_{X0}^Y f_n(Y,\sigma,0,0,\ldots,0) - f_{n-1}(X,0,\ldots,0) = 0 \tag{18}
\]
and
\[
f_n(X,\sigma_0,\ldots,\sigma_{i-1},1,0,\sigma_{i+2},\ldots,\sigma_n) = f_{n-1}(X,\sigma_0,\ldots,\sigma_{i-1},1,\sigma_{i+2},\ldots,\sigma_n) + f_{n-1}(X,\sigma_0,\ldots,\sigma_{i-1},0,\sigma_{i+2},\ldots,\sigma_n), \tag{19}
\]
for \( i = 0,\ldots,n-1 \). Upon setting new variables
\[
x_n(X) = f_n(X,0,0,\ldots,0), \quad y_n(X) = f_n(X,1,0,\ldots,0), \quad n = 0,1,2,\ldots, \tag{20}
\]
we obtain the following equation
\[
\sum_Y H_{X1}^0 x_n(Y) + \sum_Y H_{X1}^1 y_n(Y) + x_{n-1}(X) = 0, \quad n = 1,2,\ldots, \tag{21}
\]
\[
\sum_Y H_{X0}^0 x_n(Y) + \sum_Y H_{X0}^1 y_n(Y) - x_{n-1}(X) = 0, \quad n = 1,2,\ldots, \tag{22}
\]
\[
\sum_Y H_{X1}^0 x_0(Y) + \sum_Y H_{X1}^1 y_0(Y) + y_0(X) = 0 \tag{23}
\]
\[
\sum_Y H_{X0}^0 x_0(Y) + \sum_Y H_{X0}^1 y_0(Y) - y_0(X) = 0 \tag{24}
\]
\[
y_n(X) = x_{n-1}(X) + y_{n-1}(X), \quad n = 1,2,\ldots, \tag{25}
\]
which is the condition for the recursion relation (11).

We consider the simplest ASEP model again as an example to make the notations clear. Now we put \( X \in V_1 \) instead of \( V_2 \) and can set \( H_{X\sigma}^Y = (h_1)^\sigma \), where \((h_1)_0^0 = \alpha, \ (h_1)_1^0 = -\alpha \ (h_1)_1^1 = \gamma \) and \((h_1)_0^1 = -\gamma \) at the left edge. We can ignore the argument \( X \) in \( x_n \) and \( y_n \) in this notation. The equation (21)-(24) reads simply
\[
\begin{pmatrix}
\alpha & -\gamma \\
-\alpha & \gamma \\
\end{pmatrix}
\begin{pmatrix}
x_n \\
y_n \\
\end{pmatrix} = \begin{pmatrix}
x_{n-1} \\
-x_{n-1} \\
\end{pmatrix}, \quad n = 1,2,\ldots,
\]
\[
\begin{pmatrix}
\alpha & -\gamma \\
-\alpha & \gamma \\
\end{pmatrix}
\begin{pmatrix}
x_0 \\
y_0 \\
\end{pmatrix} = \begin{pmatrix}
y_0 \\
-y_0 \\
\end{pmatrix}.
\]

Therefore, we obtain
\[
x_0 = \gamma + 1, \quad y_0 = \alpha, \quad x_n = \frac{1}{\alpha} x_{n-1} + \frac{\gamma}{\alpha} y_{n+1},
\]
which is compatible with the relation from (25),
\[
y_n = x_{n-1} + y_{n-1},
\]
therefore, the wave functions in the simplest ASEP model satisfy the relation (11) as already known.

Next let us eliminate the distribution functions in eqs. (21)-(24) and see the condition including only the parameters in the boundary matrix $H$. For this sake, we introduce an auxiliary variable $t$, functions

$$
\phi(P_i; t) = \sum_{j=0}^{\infty} x_j(P_i) t^j,
$$

$$
\psi(P_i; t) = \sum_{j=0}^{\infty} y_j(P_i) t^j,
$$
vectors

$$
\vec{v}_n = (x_n(P_1), y_n(P_1), \ldots, x_n(P_s), y_n(P_s)),
$$

$$
\vec{\xi}(t) = (\phi(P_1; t), \psi(P_1; t), \ldots, \phi(P_s; t), \psi(P_s; t)),
$$

and $(2s) \times (2s)$ block diagonalized matrices

$$
E_1 = \begin{pmatrix}
    e_1 & 0 \\
    e_1 & e_1 \\
    0 & \ddots \\
    0 & e_1
\end{pmatrix},
$$

$$
e_1 = \begin{pmatrix}
    -1 \\
    0 \\
    1 \\
    0
\end{pmatrix},
$$

$$
E_2 = \begin{pmatrix}
    e_2 & 0 \\
    e_2 & e_1 \\
    0 & \ddots \\
    0 & e_2
\end{pmatrix},
$$

$$
e_1 = \begin{pmatrix}
    0 & -1 \\
    0 & 1
\end{pmatrix}.
$$

We want to solve the recursion relation (21)-(25). Equation (25) reads

$$
-t \phi(P_i; t) + (1-t) \psi(P_i; t) = y_0(P_i),
$$

and eqs. (21)-(24) mean

$$
H \vec{v}_{n+1} = -E_1 \vec{v}_n,
$$

$$
H \vec{v}_0 = -E_2 \vec{v}_0,
$$

$$
H \vec{\xi}(t) = -t E_1 \vec{\xi}(t) - E_2 \vec{\xi}(t).
$$

The initial value $y_0(P_i)$ can be determined from (28) by the determinant of the $(2s-1) \times (2s-1)$ comatrix of $H + E_2$ like

$$
y_0(P_i) = \begin{vmatrix}
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} + 1 & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} \\
    H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1} & \cdots & H_{P_i1}^{P_i0} & H_{P_i1}^{P_i1}
\end{vmatrix}.$$

7
Therefore, the condition for the recursion relation is the same as the constraint for the boundary matrix that there must be a solution $\vec{\xi}(t)$ for the simultaneous equations (26)-(29). Let us assume that we have already solved the master equation for some small $s$-dimensional matrices. Moreover, let us accept the following assumption.

Assumption: With proper constants $s_i$ and $a_i$ ($i = 1, 2, \ldots, l$), the following recursion relation is satisfied.

$$
\sum_{X=P_0, \ldots, P_s} f_n(X, 0, \ldots, 0) - \sum_{X=P_0, \ldots, P_s} f_{n+1}(X, 0, \ldots, 0, 0) = \sum_{i=1}^{l} s_i a_i^n.
$$

4 Calculation of Partition Function

To calculate physical quantities such as the density currents and concentration, we have to obtain the form of the partition function $Z_n$:

$$
Z_n = \sum_{X=P_0, \ldots, P_s} \sum_{\{\sigma_i=0,1\}} f_n(X, \sigma_0, \sigma_1, \ldots, \sigma_n).
$$

Several quantities can be extracted from this function. We calculate the partition function $Z_n$ with general $n$ exactly by means of a similar technique to that used in DDM’s and SD’s papers [4, 10]. First, let us assume that we have already solved the master equation for some small $n$’s. It is nothing but a diagonalization problem for small dimensional matrices. Moreover, let us accept the following assumption.

Assumption: With proper constants $s_i$ and $a_i$ ($i = 1, 2, \ldots, l$), the following recursion relation is satisfied.
Needless to say, the above relation should be checked in the following context. Although we have not succeeded in a general proof, we can show the above relation for specific models inductively. In the general treatment proceeded in this section, we provide that this relation is true. We prepare constants $u$ and $v$ defined by
\[
    u = \sum_{X = P_1, \ldots, P_s} f_0(X, 0) - \sum_{i} s_i a_i,
\]
\[
    v = \sum_{X = P_1, \ldots, P_s} f_0(X, 1).
\]

Let us introduce the following value $Y_n(k)$, a similar quantity to HLP’s in §2, defined by
\[
    Y_n(k) = \sum_{X \in V_s \{ \tau_i = 0, 1 \}} (1 - \tau_n)(1 - \tau_{n-1}) \cdots (1 - \tau_k) f_n(X, \tau_0, \tau_1, \ldots, \tau_n),
\]
\[
    Y_n(n+1) = \sum_{X \in V_s \{ \tau_i = 0, 1 \}} f_n(X, \tau_0, \tau_1, \ldots, \tau_n),
\]
\[
    Y_{-1}(0) = u,
\]
and auxiliary functions $L_p(\lambda)$ as
\[
    L_p(\lambda) = \sum_{n=p}^{\infty} \lambda^{n+1} Y_n(n-p), \quad p = -1, 0, 1, \ldots
\]
with an extra parameter $\lambda$. By definition, we find
\[
    L_{-1}(\lambda) = \sum_{n=-1}^{\infty} \lambda^{n+1} Y_n(n+1) = u + \sum_{n=0}^{\infty} \lambda^n Z_n.
\]

It is not difficult to prove the following relations
\[
    (1 - \lambda)L_{-1}(\lambda) - L_0(\lambda) = u + v\lambda,
\]
\[
    L_{p+1}(\lambda) - L_p(\lambda) + \lambda L_{p-1}(\lambda) = \lambda^{p+1}(Y_{p-1}(0) - Y_p(0)) = - \sum_i s_i a_i^{p-1}, \quad \text{for} \quad p \geq 0.
\]

Now, we solve the recursion relation (35) under the initial condition (34) and the condition that the first term in $L_p(\lambda)$ is proportional $\lambda^{p+1}$.

For this sake, introducing a generating function $w(x, \lambda)$ with another extra variable $x$ as
\[
    w(x, \lambda) = \sum_{p=0}^{\infty} L_{p-1} x^p,
\]
the recursion relation (35) becomes
\[
    (1 - x + \lambda x^2)w(x, \lambda) = L_{-1} + x(L_0 - L_{-1}) + \sum_{p=1}^{\infty} x^{p+1} \lambda^p \left( \sum_i s_i a_i^{p-1} \right)
\]
giving the solution
\[
L_n = \frac{\omega_1^{n+2} - \omega_2^{n+2}}{\omega_1 - \omega_2} L_{-1} + \frac{\omega_1^{n+1} - \omega_2^{n+1}}{\omega_1 - \omega_2} (L_0 - L_{-1})
\]
\[
+ \sum_i s_i \lambda \left[ \frac{\omega_1^{n+1}}{(\omega_1 - \omega_2)(\omega_1 - a_i \lambda)} \right] + \frac{\omega_2^{n+1}}{(\omega_2 - \omega_1)(\omega_2 - a_i \lambda)} + \frac{(a_i \lambda)^{n+1}}{(a_i \lambda - \omega_1)(a_i \lambda - \omega_2)} \right]
\]
(36)

with functions
\[
\omega_1 = \frac{1 - \sqrt{1 - 4 \lambda}}{2}, \quad \omega_2 = \frac{1 + \sqrt{1 - 4 \lambda}}{2}
\]

Demanding the general condition \( L_p(\lambda) \sim \lambda^{p+1} \), we obtain a simple equation
\[
-\omega_2 L_{-1} - (L_0 - L_{-1}) - \sum_{i=1}^l s_i \lambda \frac{1}{\omega_2 - a_i \lambda} = 0
\]
and the initial condition (34). Finally, we see
\[
L_{-1}(\lambda) = \left( \frac{\omega_1}{\lambda} \right)^2 \left[ u + v \lambda - \sum_{i=1}^l \frac{s_i \lambda}{\omega_2 - a_i \lambda} \right]
\]
\[
= u \left( \frac{\omega_1}{\lambda} \right)^2 + v \lambda \left( \frac{\omega_1}{\lambda} \right)^2 - \lambda \left( \frac{\omega_1}{\lambda} \right)^3 \sum_i s_i
\]
\[
-\lambda^2 \left( \frac{\omega_1}{\lambda} \right)^4 \sum_i s_i a_i - \lambda^3 \left( \frac{\omega_1}{\lambda} \right)^5 \sum_i s_i a_i^2 - \cdots.
\]

Expanding \( L_{-1}(\lambda) \) as for \( \lambda \) with helpful relations
\[
\left( \frac{\omega_1}{\lambda} \right)^m = \sum_{n=0}^{\infty} m (2n + m - 1)! \frac{(2n + m - 1)!}{n! (n + m)!} \lambda^n, \quad m = 1, 2, \ldots
\]
gives the expressions
\[
Z_n = \left[ u + v \frac{n + 1}{2n + 1} \right] Z_n^{(0)} + Z_n^{(1)},
\]
\[
Z_n^{(0)} = \frac{(2n + 2)!}{(n + 1)! (n + 2)!}, \quad Z_n^{(1)} = -\sum_{i=1}^l \frac{s_i R_n(a_i)}{a_i},
\]
(37)

with a function \( R_n(a) \) defined by
\[
R_n(a) = \sum_{m=1}^{n} \frac{(2n - m + 1)!}{(n + m)! (n - m)!} a^m.
\]
(38)

The above is the exact form of the partition functions.

Let us investigate the asymptotic behavior of \( R_n(x) \) defined in (38) with large \( n \) for later convenience. We define functions
\[
r_{n,m}(a) = (m + 2) \frac{(2m - m + 1)!}{(n + 2)! (n - m)!} a^m, \quad m = 1, 2, \ldots, n.
\]
• Region $a < 2$

It is not difficult to see that the asymptotic behavior of the function $r_{n,m}(a)$ for large $n$ is

$$r_{n,1}(a) = \frac{3}{2} a Z_n^{(0)}, \quad r_{n,m}(a) \sim m \left( \frac{a}{2} \right)^m r_{n,1}(a).$$  \hspace{1cm} (39)

Therefore, the asymptotic form of the function $R_n(a)$ for large $n$ can be written as

$$R_n(a) \sim c(a) \times Z_n^{(0)},$$  \hspace{1cm} (40)

where the function $c(a)$ is independent of $n$

• Region $a > 2$

For large $n$, because $R_n(a)$ is dominated by $\max_{1 \leq k \leq n} r_{n,k}(a)$, we obtain

$$R_n(a) \sim \frac{1}{n^{b/2}} \tau(a)^n,$$  \hspace{1cm} (41)

$$\tau(a) = \frac{1}{a^{a-1}} \left( \frac{a - 2}{a - 1} \right)^{-\frac{a-2}{a-1}} \left( 1 + \frac{a - 2}{a - 1} \right)^{1 + \frac{a-2}{a-1}}.$$  \hspace{1cm} (42)

We will make use of the above expression in the next section.

### 5 Density Current and Concentration

In this section, we calculate some physical quantities and draw some phase diagrams, which just means the diagrams of the difference of the asymptotic forms of the density current and one-point function.

First, we consider the density current

$$J = \lim_{n \to \infty} \sum_X \sum_{j \neq k} \frac{f_n(X, \sigma_0, \ldots, \sigma_{k-1}, 1, 0, \sigma_{k+1}, \ldots, \sigma_n)}{Z_n},$$

which is actually independent of $k(=0,1,\ldots,n)$ and corresponds to

$$J = \lim_{n \to \infty} \frac{Z_n^{a-1}}{Z_n}. \hspace{1cm} (43)$$

From the asymptotic form of the function $R_n(a)$, (40) and (41), we can calculate the current as follows. It must be remarked that the current does not depend on $s_i$ but only on the eigenvalues $a_i$.

• Case 1: $a_i > 2$ for some $i$'s.

Let us assume

$$a_1 > a_2 > \cdots > a_k > 2 > a_{k+1} > \cdots > a_l.$$

From the asymptotic form of $R_n(a)$, it is not so difficult to show

$$\frac{1}{J} = a_1^{\frac{a_1-2}{a_1-1}} \left( \frac{a_1 - 2}{a_1 - 1} \right)^{-\frac{a_1-2}{a_1-1}} \left( 1 + \frac{a_1 - 2}{a_1 - 1} \right)^{1 + \frac{a_1-2}{a_1-1}}.$$

We must remark $J < 1/4$ in this case.
Figure 2: Concentration \((\langle \tau_i \rangle)\) in the low density phase. \(\alpha\) and \(\beta\) correspond to those in the simplest ASEP model with \(p = 1, \gamma = \delta = 0\). This notation is also used in Figs. 3 and 4.

Figure 3: Concentration in the high density phase.

- Case 2: \(a_i < 2\) for all \(i(=1, 2, \ldots, l)\).

According to eq.(40), the partition function \(Z_n\) is proportional to \(Z_n^{(0)}\) in this case. Therefore, we can show

\[
J = \lim_{n \to \infty} \frac{Z_n^{(0)}}{Z_n} = \frac{1}{4}.
\]

Hence, the density current in this region is not so sensitive to the parameters as that in the previous region. We call this region maximal current phase [9, 10].

We can say nothing more from only the density current. However, the above former region is classified further into several phases. Let us consider the cases with two eigenvalues, i.e. \(l = 2\). In the cases with two eigenvalues, the concentration, i.e. one-point function,

\[
\langle \sigma_{n-m} \rangle_n = \frac{1}{Z_n^{(0)}} \sum_{X=P_1, \ldots, P_s} \sum_{\{\sigma_i=0,1\}} \delta_{\sigma_{n-m},1} f_n(X, \sigma_0, \sigma_1, \ldots, \sigma_n)
\]

\[
= \frac{1}{Z_n^{(0)}} \sum_{j=0}^{m} \frac{(2j)!}{j!(j+1)!} Z_{n-j-1}.
\]

(44)

separates the low and high density phases [9, 10]. The shapes of the concentrations in the low and high density and maximal current phases are shown in Figs 4 and 4, respectively. As shown in a general scheme done in [10, 19] without the mean-field approximation, systems with just two eigenvalues can undergo no other phase transition other than those in Figs 2 and 4. The problems on systems with more than three eigenvalues should be open.
Figure 4: Concentration in the maximal current phase.

6 V₂-Model

We consider the special model with \( P_i = 0,1 \) in some detail. The boundary matrix is given by 12 independent parameters \( H_{ij}^{kl} \) with \( \sum_{k,l} H_{ij}^{kl} = 0 \). The initial condition \( H\vec{v}_0 = -E_2\vec{v}_0 \) is explicitly solved as

\[
y_0(0) = \begin{vmatrix}
H_{00}^{00} & H_{00}^{10} & H_{00}^{11} \\
H_{10}^{00} & H_{10}^{10} & H_{10}^{11} - 1 \\
H_{11}^{00} & H_{11}^{10} & H_{11}^{11} + 1 
\end{vmatrix}\, y_0(0),
\]

\[
y_0(1) = \begin{vmatrix}
H_{00}^{00} & H_{00}^{01} - 1 & H_{00}^{10} \\
H_{01}^{00} & H_{01}^{01} + 1 & H_{01}^{10} \\
H_{10}^{00} & H_{10}^{01} & H_{10}^{10} 
\end{vmatrix}\, y_0(1).
\]

Upon setting the function \( m(t) \) as

\[
m(t) = \begin{vmatrix}
H_{00}^{00} - t & H_{00}^{01} & H_{00}^{10} & H_{00}^{11} & y_0(0) \\
H_{00}^{01} + t & H_{01}^{00} & H_{01}^{01} & H_{01}^{11} & -y_0(0) \\
H_{10}^{00} & H_{10}^{01} & H_{10}^{10} - t & H_{10}^{11} & y_0(0) \\
-t & 1 - t & 0 & 0 & y_0(1) \\
0 & 0 & -t & 1 - t & y_0(1)
\end{vmatrix}
\]

the condition is shown \( m(t) = 0 \) independent of \( t \), which gives 3 relations among the 12 parameters \( H_{ij}^{kl} \). As an example, we concentrate the model with

\[
H_{01}^{11} = a, \quad H_{10}^{00} = b, \quad H_{01}^{10} = p, \quad H_{01}^{01} = q, \quad H_{11}^{00} = r,
\]

and the other parameters \( H_{kl}^{ij} = 0 \) for \((i,j) \neq (k,l)\). The equation gives the relation

\[
a + q = ap, \quad (r + b)(ap - r - b) + pr = 0.
\]

For instance, the model with \( a = b = 1, p = 2, q = 1 \) and \( r = 1 + \sqrt{2} \) satisfies this condition. It is obvious that the simplest ASEP model \((a = b = 1)\) is the simplest example.

Let us consider the eigenvalue problem. In this case, we see that there are two eigenvalues \((l = 2)\) as well as the simplest ASEP model and the eigenvalues \( a_1 \) and \( a_2 \) are calculated as

\[
a_1 = \frac{1}{b + r}, \quad a_2 = 1.
\]

Therefore, we see that if the parameters satisfy \( 1/(b + r) \leq 2(>2) \), the system indicates the maximal current phase (low density phase).
7 Summary and Discussion

As we have seen, possible integrable boundary interaction should satisfy eq. (31). The density current and concentration can be expressed in terms of the partition functions exactly determined by the recursion relations (7)-(9). The extension for general $\beta$ and $\gamma$ at the right edge and $p$ and $q$ in the bulk is straightforward. Because stochastic systems are equivalent to ferromagnetic spin chains, their behavior highly depends on the boundary conditions.

We must remark several points. First, the fact that an eigenvalue $a_2$ equals to 1 originates in the choice that we take an extraction rate 1 at the right edge. Secondly, some of the readers may wonder: 

*If we hide or ignore the first site, does the system reduce to the simplest ASEP model?*

In fact, the answer is no. There are two reasons or evidences. First, we must pay attention that $a_1$ is not equal to just the sum of the probability $\sum_{ij} H_{ij}^0$ because of the conservation of probability at the left edge. Secondly, even if we focus on the simplest ASEP model, we cannot obtain the precise results by hiding the left edge site $\square$. This fact comes from the recursion relations (7)-(9). The form of $a_1$ indicates an effect of bulk correlation, though it is not so clear because we have set $p = 1$ in this case.

In general, the current $J$ of the system does not depend on the parameters $H_{X\rho}^Y$ explicitly but on the eigenvalues $a_i$. It is still unknown whether there exists an interesting model with $X \in V_s$ ($s \geq 3$), especially $X \in V_2 \otimes V_2 \otimes \cdots \otimes V_2$.

Acknowledgements

The author would like to thank the members of the theoretical physics group in Univ. of Cologne and Univ. of Bonn for the discussions, comments and their hospitality. He acknowledges R. Rauph for reading the manuscript. The useful comments on the previous version sent by G. Schütz are much appreciated. This work is financially support by DFG, SFB341(KL645/3-1) and Soryushisyogakukai.

References

[1] T.M. Liggett, *Interacting Particle Systems* (Springer-Verlag, New-York, 1985).

[2] R. Kroon, H. Fleurent and R. Sprik, Phys. Rev. E47 (1993) 2462.

[3] G.M. Schütz, Int. J. Mod. Phys. B11(1997)197.

[4] M. Doi, J. Phys. A9 (1976) 1465.

[5] M. Kandar, G. Parisi and Y. Zhang, Phys. Rev. Lett. 56 (1986) 889.

[6] For example, B.P. Lee and J.L. Cardy, J. Stat. Phys. 80 (1995) 971.

[7] J. Krug, Phys. Rev. Lett. 56 (1991) 1882.

[8] L.H. Gwa and H. Spohn, Phys. Rev. Lett. 68 (1992) 725; Phys. Rev. A46 (1992) 844.

[9] B. Derrida, E. Domany and D. Mukamel, J. Stat. Phys. 69 (1992) 667.

[10] G. Schütz and E. Domany, J. Stat. Phys. 72 (1993) 72.

[11] B. Derrida, M.R. Evans, V. Hakim and V. PASquier, J. Phys. A26 (1993) 1493.
[12] S. Sandow, Phys. Rev. E50 (1994) 2660.

[13] F. Eßler and V. Rittenberg, J. Phys. A29 (1996) 3375.

[14] R.B. Stinchcombe and G.M. Schütz, Phys. Rev. Lett. 75 (1995) 140.

[15] T. Sasamoto and M. Wadati, J. Phys. Soc. Jpn. 66 (1997) 2618.

[16] N. Rajewsky, L. Santen, A. Schadschneider and M. Schreckenberg, e-print: cond-mat/9710316

[17] H. Hinrichsen, I. Peschel and S. Sandow, J. Phys. A29 (1996) 2643; H. Hinrichsen, J. Phys. A29 (1996) 3659.

[18] F.C. Alcaraz, M. Droz, M. Henkel and V. Rittenberg, Ann. Phys. (NY) 230 (1994) 250.

[19] A.B. Kolomeisky, G.M. Schütz, E.B. Kolomeisky and J.P. Straley, to appear.