A Two-Species Exclusion Model With Open Boundaries: A use of $q$-deformed algebra

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Abstract

In this paper we study an one-dimensional two-species exclusion model with open boundaries. The model consists of two types of particles moving in opposite directions on an open lattice. Two adjacent particles swap their positions with rate $p$ and at the same time they can return to their initial positions with rate $q$ if they belong to the different types. Using the Matrix Product Ansatz (MPA) formalism, we obtain the exact phase diagram of this model in restricted regions of its parameter space. It turns out that the model has two distinct phases in each region. We also obtain the exact expression for the current of particles in each phase.

PACS number: 05.60.+w, 05.40.+j, 02.50.Ga

Key words: Asymmetric Simple Exclusion Process (ASEP), Partially Asymmetric Simple Exclusion Process (PASEP), Matrix Product Ansatz (MPA)

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I. INTRODUCTION

The stationary state properties of one-dimensional driven diffusiv e systems are cur-
cently of much research interest [1-5]. These systems exhibit very interesting cooperative
phenomena such as boundary-induced phase transitions, spontaneous symmetry breaking
and single-defect induced phase transitions which are absent in one-dimensional equilib-
rium statistical mechanics. Many physical phenomena such as hopping conductivity,
growth processes and traffic flows can also be explained by these models [6-9]. One of
the most basic model is the Asymmetric Simple Exclusion Process (ASEP), which shows
a rich behavior [10]. The ASEP is a model of particles diffusing on a lattice driven by
an external field and with hard-core exclusion. Models with more than one kind of par-
ticles have also been investigated. The ASEP in the presence of a second class particle
(impurity) has provided a framework for the study of shocks (see [5] and [9]). Another
model of this kind is the Partially Asymmetric Simple Exclusion Process (PASEP). In
this model, particles are allowed to hop both to their immediate right and left sites with
unequal rates. This model has been studied both with open boundaries [20] and in the
presence of an impurity on a ring [11]. A multi-species ASEP has also been suggested,
which seems to be a simple realization for real traffic [12].

In this paper we consider a model containing two types of particles on a lattice of length
$L$ with open boundary condition. The two types of particles, which we refer to them as " positive " and " negative " particles, move in opposite direction. The positive (negative) particles are injected (removed) from the left-most site of the lattice and are removed
(injected) from the right-most site of the lattice. Every where through the lattice, two
adjacent particles interchange their positions, unless they are both positive or negative.
The system evolves according to an stochastic dynamical rule as follows. In each in-
finitesimal time step $dt$ the following events occur at each nearest-neighbour pair of sites
$i, i + 1$ ($1 \leq i \leq L - 1$):

\[
\begin{align*}
(+) (0) &\rightarrow (0)(+) \quad \text{with rate} \quad 1 \\
(0)(-) &\rightarrow (-)(0) \quad \text{with rate} \quad 1 \\
(+)(-) &\rightarrow (-)(+) \quad \text{with rate} \quad p \\
(-)(+) &\rightarrow (+)(-) \quad \text{with rate} \quad q
\end{align*}
\]  

where $(+)$ and $(-)$ indicate a positive or a negative particle, respectively, and $(0)$ indi-
cates an empty site. Also, in each infinitesimal time step $dt$, the following events may
occur at the first ($i = 1$) and the last ($i = L$) site of the lattice:

\[
\begin{align*}
\text{At site } i = 1 \quad \left\{ \begin{array}{l}
(0) \rightarrow (+) \quad \text{with rate} \quad \alpha \\
(-) \rightarrow (0) \quad \text{with rate} \quad \beta
\end{array} \right. 
\end{align*}
\]
At site $i = L$

$\begin{align*}
(0) \rightarrow (-) & \text{ with rate } \alpha \\
(+) \rightarrow (0) & \text{ with rate } \beta
\end{align*}$

For $q = 0$, this model reduces to the model introduced in [13,14] which using simulation data and doing exact calculations has been extensively studied. These authors have shown that for certain values of the parameters $\alpha, \beta$ and $p$ the symmetry of dynamics under interchange of positive and negative particles and of their directions is spontaneously broken.

In reference [15] Alcaraz et al have studied the $N$-species stochastic models with open boundary and found their related algebras, which appear in the MPA formalism first introduced in [16]. Our model can be considered as a $N = 2$ case which will be studied in details.

The process (1) has also been considered on a closed ring in [17-19]. It has been shown that when the density of positive particles is equal to the density of negative ones, depending on the values of the parameters of the model, three phases exist: a pure phase in which one has three pinned blocks of only positive, negative particles and vacancies (where the translational invariance is spontaneously broken); a mixed phase with a non-vanishing current of particles; and a disordered phase. Here we study the effects of the open boundaries. For certain cases ($\beta = 1$ or $\alpha = \infty$) we are able to solve our model exactly and find the modified phase diagrams (in comparison with $q = 0$ case). We will show that for $\alpha = \infty$, where the system is devoid of vacancies, only two phases exist. In $\beta = 1$ limit the model has also two distinct phases in which the current of positive particles is equal to those of negative ones.

This paper is organized as follows. In section 2 we will present the exact solution of the model for the case $\alpha = \infty$ using the known results. We will also obtain the exact generating function of the partition function of the model using the Matrix Product Ansatz (MPA) and calculate the current of the particles in $\beta = 1$ limit. In the last section we will compare our results with those obtained in [13] for $q = 0$.

II. MATRIX PRODUCT SOLUTIONS

In this section we will show that the stationary probability of the model defined in (1) and (2) can be obtained using the MPA for two specific cases $\alpha = \infty$ and $\beta = 1$. According to the MPA formalism, the stationary probability $P(\{C\})$ of any configuration $\{C\}$ can be written as a matrix element of a product of non-commuting operators. Before reviewing this approach we define some notations. We introduce two occupation numbers, $\tau_i$ and $\theta_i$, for each site $i$, where $\tau_i = 1$ if site $i$ is occupied by a positive particle and $\tau_i = 0$ otherwise. Similarly, $\theta_i = 1$ if site $i$ is occupied by a negative particle and $\theta_i = 0$ otherwise. Since the process is exclusive, so that each site of the lattice can only
be occupied at most by one particle, each configuration of the system is uniquely defined by the set of occupation numbers \( \{\tau_i, \theta_i\} \). Now the normalized stationary state weight for a lattice of size \( L \) can be written as:

\[
P(\{\tau_i, \theta_i\}) = \frac{1}{Z_L} \langle W | \prod_{i=1}^{L} \{\tau_i D + \theta_i A + (1 - \tau_i - \theta_i)E\} | V \rangle.
\]

The normalization factor \( Z_L \) in the denominator of the equation (3), which plays a role analogous to the partition function in equilibrium statistical mechanics, is a fundamental quantity and can be calculated using the fact \( \sum_{\{\tau_i, \theta_i\}} P(\{\tau_i, \theta_i\}) = 1 \). Thus one finds

\[
Z_L = \sum_{\{\tau_i, \theta_i\}} \langle W | \prod_{i=1}^{L} \{\tau_i D + \theta_i A + (1 - \tau_i - \theta_i)E\} | V \rangle = \langle W | G^L | V \rangle
\]

in which \( G = D + A + E \). The operators \( D, A \) and \( E \) correspond to the presence of a positive, a negative particle, and a hole respectively. These operators with the vectors \( |V\rangle \) and \( \langle W| \) satisfy a certain algebra which will be discussed below.

### A. The limit \( \alpha \to \infty \)

In this limit, as soon as a hole appears at a boundary site, it is removed. Therefore in the steady state the lattice will be empty of holes. Now the dynamical rules given by (1) and (2) reduce to

\[
\begin{align*}
(+)(-) & \to (-)(+), \text{ with rate } p \\
(-)(+) & \to (+)(-), \text{ with rate } q \\
\text{At site } i = 1 & (-) \to (+), \text{ with rate } \beta \\
\text{At site } i = L & (+) \to (-), \text{ with rate } \beta
\end{align*}
\]

Using the MPA one obtains the following quadratic algebra for this case

\[
pDA - qAD = D + A \\
\beta \langle W | A = \langle W | \\
\beta D | V \rangle = |V\rangle.
\]

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Now if one imagine the negative particles as holes, the problem reduces to the single-species PASEP with open boundaries and equal injection and extraction rates. As we mentioned, recently the PASEP has been studies widely with open boundaries [20]. Using the results given there, we find two following phases in the thermodynamic limit ($L \to \infty$):

$I. \quad \frac{\beta}{p-q} > \frac{1}{2}$

The current of the positive particles $J_+$ is equal to the current of the negative ones $J_-$ and has its maximum value

$$J_+ = J_- = \frac{p - q}{4}. \quad (7)$$

Also the density of the positive particles $\langle \tau_i \rangle$ in the bulk has a power law behavior

$$\langle \tau_i \rangle \approx \frac{1}{2} + \frac{1}{2\pi i^{1/2}}. \quad (8)$$

The density of the negative particles $\langle \theta_i \rangle$ can be obtained using the equality $\langle \tau_i \rangle + \langle \theta_i \rangle = 1$.

$II. \quad \frac{\beta}{p-q} < \frac{1}{2}$

The current of the positive particles is again equal to the current of the negative ones and is given by

$$J_+ = J_- = \beta(1 - \frac{\beta}{p-q}). \quad (9)$$

The density profile of the positive particles is linear in the bulk which is a consequence of the superposition of shocks

$$\langle \tau_i \rangle \approx \frac{\beta}{p-q} + i(1 - 2\frac{\beta}{p-q}). \quad (10)$$

This phenomenon has also been observed in the ASEP with open boundaries when the injection and extraction rates become equal [10].
Another limit which can be solved using the MPA formalism exactly is \( \beta = 1 \). The operators and vectors satisfy the following algebra

\[
pDA - qAD = \alpha(D + A) \\
DE = \alpha E \\
EA = \alpha E \\
E|V\rangle = |V\rangle \\
D|V\rangle = \alpha|V\rangle \\
\langle W|E = \langle W| \\
\langle W|A = \alpha\langle W|.
\]

Following [13] one can choose

\[
E = |V\rangle\langle W| , \quad \langle V|W\rangle = 1. \tag{12}
\]

Then the algebra (11) can be written as

\[
\left(\frac{p}{\alpha}\right)DA - \left(\frac{q}{\alpha}\right)AD = D + A \\
D|V\rangle = \alpha|V\rangle \\
\langle W|A = \alpha\langle W|.
\]

This algebra is very similar to the algebra associated with the PASEP [19,20]. Here we adopt the same representation proposed in [19]. One can easily check that the following representation satisfy (12) and (13)

\[
D = \frac{\alpha}{p - q} \begin{pmatrix}
1 + a\sqrt{c_1} & 0 & 0 & \ldots \\
0 & 1 + a\left(\frac{q}{p}\right)\sqrt{c_2} & 0 & \ldots \\
0 & 0 & 1 + a\left(\frac{q}{p}\right)^2\sqrt{c_3} & \ldots \\
0 & 0 & 0 & 1 + a\left(\frac{q}{p}\right)^3 & \ldots \\
\vdots & \vdots & \vdots & \ddots & \ddots 
\end{pmatrix}, \quad A = D^T, \quad E = |0\rangle\langle 0|. \tag{14}
\]

Where the superscript \( T \) indicates the transpose,
\[ c_n = (1 - \left( \frac{q}{p} \right)^n) (1 - a^2 \left( \frac{q}{p} \right)^{n-1}) \quad a = p - q - 1, \quad (15) \]

\[ \langle 0 | = [1000 \ldots] \text{ and } |0\rangle = \langle 0 |^T. \] Using the matrix algebra given by (12) and (13) we find the following expressions for the current of the positive and the negative particles in the stationary state

\[ J_+ = \frac{\langle W|G^{i-1}(pDA - qAD + DE)G^{L-i-1}|V\rangle}{\langle W|G^L|V\rangle} = \alpha \frac{\langle W|G^{L-1}|V\rangle}{\langle W|G^L|V\rangle}, \]

\[ J_- = \frac{\langle W|G^{i-1}(pDA - qAD + EA)G^{L-i-1}|V\rangle}{\langle W|G^L|V\rangle} = \alpha \frac{\langle W|G^{L-1}|V\rangle}{\langle W|G^L|V\rangle}. \quad (16) \]

As can be seen from (16), the currents are site-independent (as it should be in the stationary state), equal and given by the matrix element of powers of \( G \). In what follows we will introduce a generating function to calculate the matrix element of all powers of \( G \) between the vectors \( |V\rangle \) and \( \langle W| \).

Define a generating function

\[ f(\lambda) := \sum_{L=1}^{\infty} \lambda^{L-1} \langle W|G^L|V\rangle. \quad (17) \]

The convergence radius of this formal series, \( R \), is proportional to the current of particles given by (16) in the thermodynamic limit

\[ R = \lim_{L \to \infty} \frac{\langle W|G^{L-1}|V\rangle}{\langle W|G^L|V\rangle}. \quad (18) \]

On the other hand, the radius of convergence is the absolute value of the nearest singularity of \( f(\lambda) \) to the origin. Once we obtain the singularities of the function \( f(\lambda) \), we can calculate the current of particles and distinguish the phases.

Using (12) and (13) one can expand the expression \( \langle W|G^L|V\rangle \) as

\[ \langle G^L \rangle := \langle W|G^L|V\rangle = \sum_{r \geq 0} \sum_{j_0, j_r \geq 0} \sum_{j_1, m_1, \ldots, j_r, m_r > 0} \sum_{j_0 + m_1 + j_1 + \ldots + m_r + j_r = L} \langle W|C^{j_0}E^{m_1}C^{j_1} \ldots E^{m_r}C^{j_r}|V\rangle \quad (19) \]

where \( C := D + A \). Noting that \( E^m = E \), after some computation, we obtain
\( (G^L) = (C^L) + \sum_{r=1}^{L} \sum_{j_0, j_r \geq 0}^{j_0 \to j_0 + \ldots + j_r \leq L-r} \frac{(L - 1 - j_0 - \ldots - j_r)!}{(r - 1)!(L - r - j_0 - \ldots - j_r)!} \langle C^{j_0} \rangle \ldots \langle C^{j_r} \rangle \) \hspace{1cm} (20)

and also

\[
f(\lambda) = \sum_{L=1}^{\infty} \lambda^{L-1} (G^L) = \frac{(1 - \lambda^{-1}) + \lambda^{-2}(1 + \lambda) \sum_{n=0}^{\infty} \lambda^{n+1} \langle C^{n} \rangle}{1 - \sum_{n=0}^{\infty} \lambda^{n+1} \langle C^{n} \rangle}.
\]

It is known that the expression \( g(\lambda) := \sum_{n=0}^{\infty} \lambda^{n+1} \langle C^{n} \rangle \) can be written explicitly in terms of the basic \( q \)-hypergeometric function (see [19] and references therein)

\[
g(x(\lambda)) = x^{(p-q)} \left( \frac{q}{p} \right)^{2 \alpha} \left( \frac{q}{p} \right)^{\infty} \left( \frac{q}{p} \right)^{\infty} \left( \alpha, ax, ax \right)_{\infty} \sum_{r=0}^{\infty} \frac{\sum_{n=0}^{\infty} \sum_{k=0}^{n} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}}{\lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}} \sum_{n=0}^{\infty} \frac{\sum_{k=0}^{n} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}}{\lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}
\]

\[
\sum_{n=0}^{\infty} \frac{\sum_{k=0}^{n} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}}{\lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}} \sum_{n=0}^{\infty} \frac{\sum_{k=0}^{n} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}}{\lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}
\]

in which \( x(\lambda) = \frac{1}{2} \{ \frac{p-q}{\alpha} - 2 - \sqrt{\frac{(p-q)^2}{\alpha^2} - 4 \frac{p^2}{\alpha^2}} \} \). The quantities \((z; q)_n\) and \((z; q)_\infty\) are defined as

\[
(z; q)_n = \begin{cases} 1, & \text{if } n = 0, \\ (1 - z)(1 - zq)(1 - zq^2) \cdots (1 - zq^{n-1}), & \text{if } n > 0, \end{cases}
\]

\[
(z; q)_\infty = \prod_{n=0}^{\infty} (1 - zq^n).
\]

Lastly, the basic \( q \)-hypergeometric function is defined by the series

\[
\sum_{n=0}^{\infty} \frac{\sum_{k=0}^{n} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}}{\lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}} \sum_{n=0}^{\infty} \frac{\sum_{k=0}^{n} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}}{\lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}} \lambda^{n+r} C_{n}^{r}(\lambda) q^{\alpha}
\]

which tends to the usual hypergeometric series as \( q \to 1 \). The \( 2\phi_1 \) series converges when \( 0 < |q| < 1 \) and \( |z| < 1 \) [20]. In this paper the convergence condition of (22) is \( q < p \); therefore, without losing the generality, we limit ourselves to this region.

As we mentioned, the singularities of \( f(\lambda) \) specify the phase diagram of the model. From the expression (21), we see that there are two possible sources for the singularities: the singularities of \( g(x(\lambda)) \) and a zero of the denominator of (21). First we consider the singularities of \( g(x(\lambda)) \). From (22) one can see that \( g(x(\lambda)) \) has two singularities: \( \lambda_1 = \frac{p-q}{4\alpha} \) which is a square root singularity and \( \lambda_2 = \frac{p-q-1}{\alpha(p-q)} \) which is a simple root. In order to
discuss the zeros of the denominator of $f(\lambda)$, we use the same assumption proposed in [19]. In the convergence region of (22) i.e. $q < p$, for $0 \leq x \leq 1$ the function $g(x)$ satisfies $g'(x) > 0$. It means that the function $g(x)$ increases monotonically from 0 to $g(1)$ when $0 \leq x \leq 1$; therefore, the equation $g(x(\lambda_3)) = 1$ (which gives the zeros of the denominator of (21)) has only one root in this region. Comparing the absolute value of the singularities $\lambda_1$, $\lambda_2$ and $\lambda_3$, one can easily find the following results:

I) For $p - q \geq 2$ the radius of convergence (18) of the formal series (17) is equal to $R = \lambda_3 < \lambda_1, \lambda_2$ which is the solution of the equation $g(x(\lambda_3)) = 1$. Since $\lambda_3$ is a simple pole, we expect that $Z_L$ behaves asymptotically ($L \to \infty$) as $\lambda_3^{-L}$. The current of the particles (16) can also be obtained

$$J_+ = J_- = \alpha \lambda_3$$  \hspace{1cm} (25)

II) For $p - q < 2$ two different situations may occur. In the region specified by $g(1) \leq 1$ and $p - q < 2$, we find $R = \lambda_1 = \frac{p-q}{4\alpha}$ and the current of particles to be

$$J_+ = J_- = \frac{p-q}{4}$$  \hspace{1cm} (26)

In the region $g(1) > 1$, it turns out that $R = \lambda_3 < \lambda_1, \lambda_2$ which is again the solution of the equation $g(x(\lambda_3)) = 1$. The partition function $Z_L$ again behaves as $\lambda_3^{-L}$ and the current of particles in this case can be obtained from (25). The boundary of these two recent phases will be specified by

$$g(1) = \frac{(p-q)}{\alpha} \frac{\binom{q}{p}}{(p-q-1) \binom{q}{p}^2}_\infty 2\phi_1 \left[ p-q-1, p-q-1; \frac{q}{p}, \frac{q}{p} ; \frac{q}{p} \right] = 1$$ \hspace{1cm} (27)

In Fig.1 we have plotted the phase diagram of our model in $\beta = 1$ limit both for $q \neq 0$ (the left diagram) and $q = 0$ (the right diagram). As we mentioned in section (2) for $\alpha = \infty$, the line $p - q \geq 2$ is the line of shock configurations. The bold lines in Fig.1 mark these lines.
FIGURES

FIG. 1. Plot of the phase diagrams for \( q = 0 \) (the right diagram) and \( q \neq 0 \) (the left diagram) in \( \beta = 1 \) limit.

III. COMPARISON AND CONCLUDING REMARKS

In this paper we studied a generalized two-species exclusion model with open boundaries. The positive particles are supplied at the left end of the chain and they leave it at the right end. Similarly, the negative particles are supplied at the right end and they leave the system at the left end. As soon as a positive and a negative particle meet each other (the positive particle is supposed to be in the left hand side of the negative particle), they interchange their positions with rate \( p \). At the same time they may go to their initial positions with rate \( q \). In \( q = 0 \) limit this model reduces to the one studied in [13]. Using the MAP formalism, our model has been studied in two different limits (\( \alpha = \infty \) and \( \beta = 1 \)) and the corresponding phase diagrams obtained. It has been shown that all the phases are symmetric in which the current of the positive and negative particles are equal. One can easily check that for \( q = 0 \) all the results obtained here reduce to those obtained in [13]. In comparison with [13], as can be seen in Fig.1, the phase diagram of the model has been modified.

The study of the whole parameters space of the model proposed in this paper is still an open problem. Using the mean field approximation and simulation data, the authors have shown that in \( q = 0 \) limit this model has also asymmetric phases where the current of the positive and negative particles become different. It will be interesting to study the structure of asymmetric phases of this model which may occur for the certain values of the parameters \( \alpha, \beta, p \) and \( q \).

Acknowledgement:
I would like to thank V. Karimipour for reading the manuscript.
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