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Partially asymmetric simple exclusion model in the presence of an impurity on a ring

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Abstract. We study a generalized two-species model on a ring. The original model (Mallick K 1996 *J. Phys. A: Math. Gen.* **29** 5375) describes ordinary particles hopping exclusively in one direction in the presence of an impurity. The impurity hops with a rate different from that of ordinary particles and can be overtaken by them. Here we let the ordinary particles also hop backward with rate q. Using the matrix product ansatz we obtain the relevant quadratic algebra. A finite-dimensional representation of this algebra enables us to compute the stationary bulk density of the ordinary particles, as well as the speed of impurity on a set of special surfaces of the parameter space. We will obtain the phase structure of this model in the accessible region and show how the phase structure of the original model is modified. In the infinite-volume limit this model presents a shock in one of its phases.

1. Introduction

Recently, much attention has been focused on one-dimensional reaction–diffusion processes. These models can describe many physical phenomena such as hopping conductivity, growth processes and traffic flows [2–4]. They are also of interest from the mathematical point of view due to their relation to integrable quantum chain Hamiltonians [5, 6]. The simplest model of this kind is the asymmetric simple exclusion process (ASEP) with open boundaries [7]. This model comprises particles which jump independently to their right with hard core repulsion along a one-dimensional lattice. The open boundary conditions mean that particles are injected at one end of the lattice and are removed at the opposite end. This model exhibits a shock structure in the density profile of particles. In periodic boundary conditions, the microscopic location of the shock can be identified by defining a second-class particle (impurity). The ASEP in the presence of an impurity on a ring has been studied in the two following cases:

(1) In the first case, the single impurity hops in the opposite direction relative to the ordinary particles [8, 9]. In this case a first-order phase transition between a low-density and a traffic-jam phase is observed.

(2) In the second case, the impurity moves in the same direction as the ordinary particles [1,18]. The phase diagram of this model consists of six distinctive phases (I)–(VI) in which two of them are symmetric to other phases under a charge conjugation and reflection symmetry. The authors have shown that one phase exists in the system in which the impurity causes a shock.

Another example of such driven diffusive systems is the partially asymmetric simple exclusion process (PASEP). In this model the particles are allowed to jump both to their immediate right (with rate p) or left (with rate q) site, if the target site is not already occupied. This model has been extensively studied both with open boundaries and on a ring [10].

In this paper we will study the effects of the presence of a single impurity on the PASEP on a ring. Here, the ordinary particles can hop to their immediate right (left) site, provided that it is empty, with rate 1 $(q \leqslant 1)$. The single impurity can only hop to its immediate right site (if it is not already occupied) with rate α ($\leqslant$1) and can be exchanged from the left with the ordinary particles with rate β ($\leqslant$1). For $q = 0$ this model reduces to the model (2) as discussed above. Using the matrix product ansatz (MPA) introduced in [11], we obtain the relevant quadratic algebra which has both finite- and infinite-dimensional representations. For simplicity, we adopt a finite-dimensional representation of the algebra and carry out all the calculations using a grand canonical ensemble in which the population of ordinary particles can fluctuate. By adjusting the fugacities of the ordinary particles and of the holes, one can produce some fixed densities for them. Although the finite-dimensional representation restricts us to the region under the surface $\alpha + \beta + q = 1$ in the three-dimensional parameter space, nevertheless we shall find the exact phase structure and calculate precisely the density profile of ordinary particles and the speed of impurity in this region. With these exact results, we will show that three phases exist in this region. In two of them, which are symmetric to each other under a charge conjugation and reflection symmetry, the density profile of particles has an exponential behaviour. We will determine the relevant correlation lengths in these phases and the critical values of the rates that characterize the divergence of these correlation lengths. In the third phase the density profile of the ordinary particles is linear which is a signature of a shock.

This paper is organized as follows. In section 2 we will describe the model. In section 3 we will write the weights of the configurations in the stationary state in terms of a trace of $L+1$ non-commuting matrices and obtain the quadratic algebra. In section 4 we will introduce all possible representations of the quadratic algebra and discuss different phases in the accessible region of the phase space. In section 5, using one- and two-dimensional representations of the algebra we will obtain some exact results for an infinite system. In the last section we will compare our results with those obtained in [1] for $q = 0$.

2. The model

The model proposed here contains two species of particles on a closed ring of $L+1$ sites which are labelled from 1 to $L + 1$. We specify each configuration of the system by an $L + 1$-tuple $(\tau_1, \tau_2, \ldots, \tau_{L+1})$, where $\tau_i = 1$ if site i is occupied with a particle of kind 1, $\tau_i = 2$ if it is occupied with a particle of kind 2, and $\tau_i = 0$ if site i is empty. There are M particles of kind 1, and only one particle of kind 2 on the ring. We will refer to them as ordinary particles and impurity, respectively.

The system evolves under stochastic dynamics. The possible exchanges between two adjacent sites during a time interval $\mathrm{d}t$ are as follows:

$$
\begin{aligned}
10 &\rightarrow 01 && \text{with} \quad \text{rate } 1\\
01 &\rightarrow 10 && \text{with} \quad \text{rate } q\\
20 &\rightarrow 02 && \text{with} \quad \text{rate } \alpha\\
12 &\rightarrow 21 && \text{with} \quad \text{rate } \beta.
\end{aligned}
$$

The space of configuration is connected. Each configuration can evolve into any other and, therefore, it has a unique stationary state [19]. As we mentioned above, we will perform all the calculations in the grand canonical ensemble and let the number of ordinary particles fluctuate around a mean value. The above process can be mapped onto the one introduced in [12] by interchanging the impurity and vacancies ($2 \Longleftrightarrow 0$). It can also be considered as a special case of the three-species diffusion problems introduced in [13].

3. The stationary measure and the quadratic algebra

According to the matrix product formalism, the stationary probability $P(\{\tau\})$ of any configuration $\{\tau\}$ can be written as a trace of a product of non-commuting operators. Since this model is translationally invariant, one can always keep the single impurity at site $L + 1$ and write the normalized weight $P(\{\tau\})$ in terms of three operators D, E and A:

$$P(\{\tau\}) = P(\{\tau_1, \tau_2, \ldots, \tau_L, \tau_{L+1} = 2\}) = \frac{1}{Z_L} \operatorname{Tr}\left[\prod_{i=1}^{L}(x\tau_i D + y(1-\tau_i)E)A\right]. \tag{1}$$

The non-zero real variables, x and y, are the fugacities of ordinary particles and vacancies, respectively. In the grand canonical ensemble approach, one must choose the value of the fugacities to fix the density of ordinary particles to be $\rho = \frac{M}{L}$. Although it would be sufficient to introduce only one fugacity (since the total number of sites '$L + 1$' is fixed), we use both of them to make the symmetry between ordinary particles and vacancies more apparent. The normalization factor Z_L in the denominator of equation (1), which plays a role analogous to the partition function in equilibrium statistical mechanics, is a fundumental quantity and can be calculated using the fact $\sum_{\{\tau\}} P(\{\tau_1, \ldots, \tau_L, \tau_{L+1}\}) = 1$. Thus one finds

$$Z_L = \sum_{\text{all configurations}} \operatorname{Tr}\left[\prod_{i=1}^{L}(x\tau_i D + y(1-\tau_i)E)A\right] = \operatorname{Tr}(C^L A) \tag{2}$$

in which $C = xD + yE$. The operators D, E and A satisfy the following quadratic algebra:

$$DE - qED = D + E \tag{3}$$

$$\beta DA = A \tag{4}$$

$$\alpha AE = A. \tag{5}$$

Following [14], we write A as $|V\rangle\langle W|$, which converts the above relations into

$$DE - qED = D + E \tag{6}$$

$$D|V\rangle = \frac{1}{\beta}|V\rangle \tag{7}$$

$$\langle W|E = \frac{1}{\alpha}\langle W|. \tag{8}$$

With this assumption, the calculation of $\operatorname{Tr}(\ldots)$ in expression (2) reduces to the calculation of a matrix element

$$Z_L = \langle W|C^L|V\rangle. \tag{9}$$

In the next section we will investigate all possible representations of (6)–(8).

4. Representations of the quadratic algebra

In [15] the Fock representation of the most general quadratic algebra has been obtained. It has been shown that in order to have a finite-dimensional representation of certain quadratic algebras, the parameters of the model, say α, β and q in (6)–(8), should satisfy a set of constraints.

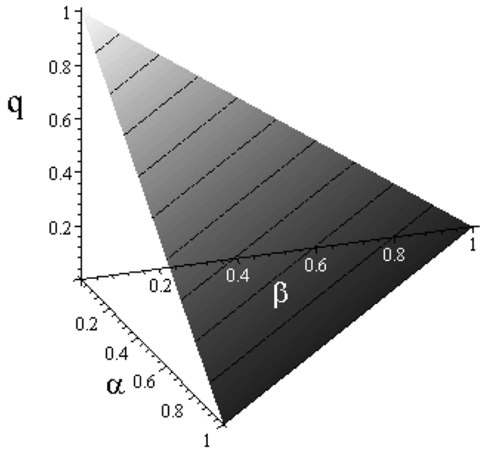

Figure 1. Plot of equation (11).

The algebra (6)–(8) has a one-dimensional representation for $\alpha, \beta, q < 1$, where the operators D, E and A are represented by real numbers. Here the vectors $|V\rangle$ and $\langle W|$ can be discarded and one is dealing with a scalar product state in (9). This representation exists if

$$D = \frac{1}{\beta} \qquad E = \frac{1}{\alpha} \qquad A = 1 \tag{10}$$

and the following constraint holds:

$$\alpha + \beta + q = 1. \tag{11}$$

In figure 1 we have ploted (11) in the three-dimensional parameters space.

For the finite-dimensional representations, one can easily check that the following matrices [16]:

$$D = \frac{1}{1-q}\begin{pmatrix} 1+a & 0 & 0 & \cdot & \cdot \\ 0 & 1+aq & 0 & \cdot & \cdot \\ 0 & 0 & 1+aq^2 & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & 1+aq^{n-2} & 0 \\ \cdot & \cdot & 0 & 0 & 1+aq^{n-1} \end{pmatrix} \tag{12}$$

$$E = \frac{1}{1-q}\begin{pmatrix} 1+\frac{1}{a} & 0 & 0 & \cdot & \cdot \\ 1 & 1+\frac{1}{aq} & 0 & \cdot & \cdot \\ 0 & 1 & 1+\frac{1}{aq^2} & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & 1+\frac{1}{aq^{n-2}} & 0 \\ \cdot & \cdot & 0 & 1 & 1+\frac{1}{aq^{n-1}} \end{pmatrix} \tag{13}$$

form an n-dimensional representation of (6), where a is an arbitrary parameter. The vectors $|V\rangle$ and $\langle W|$ are also found to be

$$|V\rangle = \begin{pmatrix} 1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{pmatrix} \qquad |W\rangle = \begin{pmatrix} 1 \\ \omega_2 \\ \omega_3 \\ \cdot \\ \cdot \\ \omega_n \end{pmatrix} \qquad \omega_i = \prod_{j=0}^{i-2} \frac{1}{a}\left(\frac{1}{q^{n-1}} - \frac{1}{q^j}\right) \qquad i = 2, \ldots, n. \tag{14}$$

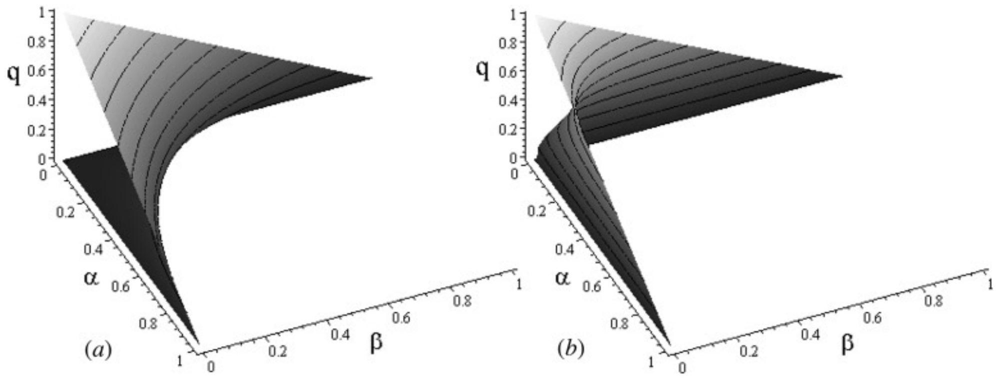

Figure 2. Plots of equation (16) for $n = 2$ (*a*) and $n = 5$ (*b*).

The parameter a is then fixed as follows:

$$a = \frac{1-q-\beta}{\beta} = \frac{1}{\frac{1-q-\alpha}{\alpha}q^{n-1}} \tag{15}$$

where $\alpha, \beta, q < 1$. Equation (15) then provides the following constraint between the parameters α, β and q:

$$\left(\frac{1-q-\beta}{\beta}\right)\left(\frac{1-q-\alpha}{\alpha}\right) = q^{1-n}. \tag{16}$$

Note that for $n = 1$ the above constraint reduces to (11). Using (16) it can be verified that for $q < 1$, the region of the phase space which is accessible by the totality of all finite-dimensional ($n \geqslant 2$) representations is

$$\alpha + \beta + q < 1. \tag{17}$$

In figure 2 we have plotted (16) for two values of n. One can see that as the dimension of representation increases from 2, the two-dimensional surface (16) begins to approach towards the q axis. Therefore, the finite-dimensional representation of the algebra (6)–(8) allows us to derive exact results for this model only on some special surfaces given by (16). However, using the same conjecture proposed in [16], one can introduce a kind of analytical continuation to obtain results valid in the whole accessible region given by (17).

As we will see in the next section the speed of impurity and density profile of ordinary particles on the ring depend on the asymptotic behaviour of the expression (9) in thermodynamic limit ($L, M \longrightarrow \infty$, the density $\rho = \frac{M}{L}$ being constant). On the other hand, the asymptotic behaviour of Z_L in this limit is governed by the largest eigenvalue of C. In what follows we will show that in the region specified by (17), Z_L can possess only three different asymptotic values in the thermodynamic limit, i.e. only three phases can exist in which the speed of impurity and density profile of ordinary particles are given by different expressions. Noting that the fugacity of ordinary particles x and vacancies y remain constant in the large L limit, the eigenvalues ξ_i of

$$C = xD + yE$$
$$= \frac{1}{1-q}\begin{pmatrix} (x+y)+xa+\frac{y}{a} & 0 & \cdot & \cdot \\ y & (x+y)+xaq+\frac{y}{aq} & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & y & (x+y)+xaq^{n-1}+\frac{y}{aq^{n-1}} \end{pmatrix} \tag{18}$$

can readily be computed

$$\xi_i = \frac{1}{1-q}\left\{(x+y) + xaq^{i-1} + \frac{y}{aq^{i-1}}\right\} \qquad i = 1, \ldots, n. \tag{19}$$

We notice that all the eigenvalues of C lie on the curve [16]

$$z \longrightarrow \frac{1}{1-q}\left((x+y) + xz + \frac{y}{z}\right)$$

in which $z = a, aq, \ldots, aq^{n-1}$. Since the fugacities x and y are positive, this implies that the largest eigenvalue $\xi_{\max}$ of C takes one of the following values:

(I) $\xi_{\max} = \xi_1$, if $\xi_1 > \xi_n$, or, equivalently, $x(\frac{1-q-\beta}{\beta}) > y(\frac{1-q-\alpha}{\alpha})$

(II) $\xi_{\max} = \xi_n$, if $\xi_n > \xi_1$, or, equivalently, $x(\frac{1-q-\beta}{\beta}) < y(\frac{1-q-\alpha}{\alpha})$

(III) $\xi_{\max} = \xi_1 = \xi_n$, if $\xi_1 = \xi_n$, or, equivalently, $x(\frac{1-q-\beta}{\beta}) = y(\frac{1-q-\alpha}{\alpha})$.

As we mentioned above these three different cases correspond to different phases in the region (17), distinguished by different expressions for the speed of impurity and density profile. By using (18) one can see that in the regions (I) and (II) C is diagonalizable, therefore, we expect that all correlation functions of form $\langle \tau_{i_1} \ldots \tau_{i_{L+1}} \rangle$ depend exponentially on the distances involved. In these regions one obtains the following asymptotic form for Z_L in the thermodynamic limit [16]:

$$Z_L = \langle W|C^L|V\rangle \simeq \xi_i^L \langle W|\xi_i\rangle\langle\xi_i|V\rangle$$

in which $i = 1$ and n for the phases (I) and (II), respectively. The vector $|\xi_i\rangle$ ($\langle\xi_i|$) is the corresponding right (left) eigenvector of C. In the region (III) the eigenvalues of C coincide

$$\xi_k = \xi_{n-k+1} = \frac{1}{1-q}\left\{(x+y) + y\left(\frac{1-q-\alpha}{\alpha}\right)(q^{k-1} + q^{n-k})\right\} \qquad k = 1, \ldots, n. \tag{20}$$

In this case, since C has an off-diagonal line (see (18)), it is not diagonalizable. Hence it implies an algebraic behaviour of all correlation functions (see discussions in [17]). One can also find the following expression for Z_L for large system sizes in this phase [16]:

$$Z_L = \langle W|C^L|V\rangle \simeq L\xi^L$$

in which $\xi = \xi_1 = \xi_n$. In the next section we will show these explicitly for a two-dimensional representation.

The process is invariant when the direction of motion is reversed and the following transformations are applied:

Particle of kind 1	$\longrightarrow$	Particle of kind 0 (Vacancy)
Site number i	$\longrightarrow$	Site number $L + 1 - i$
ρ	$\longrightarrow$	$1 - \rho$
α	$\longrightarrow$	β.

Now considering that the interchange of x and y is equivalent to the exchange of the density of ordinary particles and vacancies, (I) is symmetric to (II) under these transformations.

The algebra (6)–(8) also has infinite-dimensional representations [13, 15] and by using them one has access to the entire phase space without any constraints on the parameters. Since the calculations for these representations seem to be very difficult, we shall adopt one and two-dimensional representations to study the general behaviour of some interesting quantities, such as the density profile of ordinary particles and the speed of impurity in different phases.

5. One- and two-dimensional representations. Exact results

As mentioned in the previous section, using n-dimensional representations ($n \geqslant 2$), only the region $\alpha + \beta + q < 1$ is accessible, where three phases exist. One-dimensional representation (10) limits us to that part of phase space given by the constraint (11). On this two-dimensional surface, the partition function (9) has a simple form

$$Z_L = \left(\frac{x}{\beta} + \frac{y}{\alpha}\right)^L. \tag{21}$$

The mean value of density of the ordinary particles which is defined by

$$\rho = \frac{x}{L}\frac{\mathrm{d}}{\mathrm{d}x}\ln Z_L \tag{22}$$

can easily be evaluated

$$\rho = \frac{\frac{x}{\beta}}{\frac{x}{\beta} + \frac{y}{\alpha}}. \tag{23}$$

If ρ_i denotes the expectation that site i is occupied with an ordinary particle in the stationary state, knowing that the only impurity is at site $L + 1$, we have

$$\rho_i = x\frac{\mathrm{Tr}(C^{i-1}DC^{L-i}A)}{\mathrm{Tr}(C^L A)} = x\frac{\langle W|C^{i-1}DC^{L-i}|V\rangle}{\langle W|C^L|V\rangle}. \tag{24}$$

Consequently, using (10) and (23), we are able to evaluate the density profile of ordinary particles in this case

$$\rho_i = \rho. \tag{25}$$

In figure 3 we have plotted the phase diagram of the model for a constant q. The accessible region (17) lies under the line $\alpha + \beta = 1 - q$. On this line each configuration has the same stationary probability and mean field results become exact. In the stationary state, the speed of impurity v can be expressed as

$$v = y\alpha\frac{\mathrm{Tr}(EC^{L-1}A)}{\mathrm{Tr}(C^L)} - x\beta\frac{\mathrm{Tr}(C^{L-1}DA)}{\mathrm{Tr}(C^L)} = (y - x)\frac{Z_{L-1}}{Z_L} \tag{26}$$

when use has been made of the algebraic relations (6)–(8). Using (21), (23) and (26) the speed of impurity is found to be

$$v = \alpha - (1 - q)\rho. \tag{27}$$

One may also note that for $\alpha > (1 - q)\rho$, (27) becomes negative, i.e. the impurity starts moving backward. This can easily be understood from the fact that whenever an ordinary particle appears behind the impurity, it overtakes the impurity while pushing it backward (see section 2). Thus, when the density of ordinary particles exceeds a critical value $\rho_c = \frac{\alpha}{1-q}$, a macroscopic negative current of impurity evolves in the system.

Now we will consider a two-dimensional representation. The following matrices:

$$D = \begin{pmatrix} \frac{1}{\beta} & \frac{\mathrm{i}}{\sqrt{q}} \\ 0 & \frac{\beta+q}{\beta} \end{pmatrix} \qquad E = \begin{pmatrix} \frac{1}{\alpha} & 0 \\ \frac{\mathrm{i}}{\sqrt{q}} & \frac{\alpha+q}{\alpha} \end{pmatrix} \tag{28}$$

with the vectors

$$|V\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |W\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{29}$$

satisfy (6)–(8), if the following relation holds:

$$(q + \alpha)(q + \beta) = q. \tag{30}$$

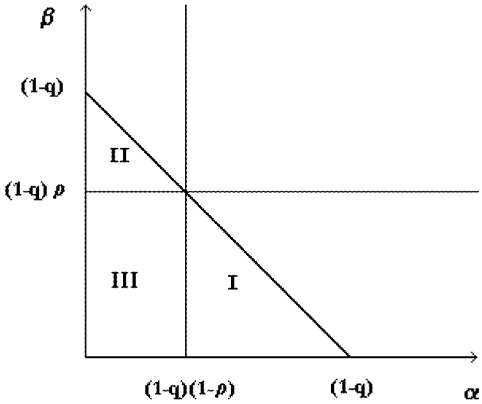

Figure 3. The phase diagram.

For $n = 2$, this representation is equivalent to (12)–(14) and (30) concides with (16). As we saw, the properties of the matrix

$$C = \begin{pmatrix} \frac{x}{\beta} + \frac{y}{\alpha} & \frac{x\mathrm{i}}{\sqrt{q}} \\ \frac{y\mathrm{i}}{\sqrt{q}} & x(\frac{\beta+q}{\beta}) + y(\frac{\alpha+q}{\alpha}) \end{pmatrix} \tag{31}$$

is of prime importance in determining the phase structre of the model. The eigenvalues of C can easily be computed

$$\xi_1 = \frac{x}{\beta} + \left(1 + \frac{q}{\alpha}\right) y \qquad \xi_2 = \left(1 + \frac{q}{\beta}\right) x + \frac{y}{\alpha}.$$

These eigenvalues also coincide with those obtained from (19) for $n = 2$. For $\xi_1 \neq \xi_2$, one can introduce

$$U = \frac{1}{\sqrt{\frac{\mathrm{i}}{\sqrt{q}}(y(\frac{1-q-\alpha}{\alpha}) - x(\frac{1-q-\beta}{\beta}))}} \begin{pmatrix} \frac{x\mathrm{i}}{\sqrt{q}} & -y\frac{1-q-\alpha}{\alpha} \\ \frac{\mathrm{i}}{\sqrt{q}} & -\frac{1-q-\beta}{\beta} \end{pmatrix} \tag{32}$$

to diagonalize C

$$UCU^{-1} = \begin{pmatrix} \xi_1 & 0 \\ 0 & \xi_2 \end{pmatrix}$$

and using (9) and (29) we obtain the following expresion for Z_L:

$$Z_L = \frac{x(\frac{1-q-\beta}{\beta})\xi_1^L - y(\frac{1-q-\alpha}{\alpha})\xi_2^L}{x(\frac{1-q-\beta}{\beta}) - y(\frac{1-q-\alpha}{\alpha})}. \tag{33}$$

In the thermodynamic limit, two cases can be distinguished. The first case, corresponding to phase (I), is specified with $\xi_1 > \xi_2$, where the first term in (33) becomes dominant. The mean density of ordinary particles (22) can be evaluated as

$$\rho = \frac{\frac{x}{\beta}}{\frac{x}{\beta} + y(1 + \frac{q}{\alpha})}. \tag{34}$$

The inequality $\xi_1 > \xi_2$ can be written in terms of ρ as

$$\alpha > (1-q)(1-\rho)$$

which with $\alpha + \beta + q < 1$ define the boundaries of the phase (I) (see figure 3). In the $q \to 0$ limit, this phase corresponds to phase (VI) of the model studied in [1]. Using (24), (28)–(30), (32) and (34) we obtain

$$\rho_1 = 1 - \frac{1}{q+\alpha}(1-\rho) \qquad \rho_L = \rho. \tag{35}$$

The density profile decreases exponentially from ρ_1 to ρ_L. One can define a characteristic length measuring the range of the effect of the impurity

$$\xi^{-1} = \ln \frac{q+\alpha}{1+\rho(q-1)}. \tag{36}$$

Note that the correlation length diverges as $\rho \longrightarrow 1 - \frac{\alpha}{1-q}$. For $L \gg \xi$ the density profile of the ordinary particles is of the form

$$\rho_i = c_1 \mathrm{e}^{\frac{-\mathrm{i}}{\xi}} + c_2 \mathrm{e}^{\frac{\mathrm{i}-L}{\xi}} + c_3 \tag{37}$$

in which

$$c_1 = \frac{-xy(\frac{1-q-\alpha}{\alpha})(\frac{1-q-\alpha}{\alpha} - \frac{1-q-\beta}{\beta})}{(y\frac{1-q-\alpha}{\alpha} - x\frac{1-q-\beta}{\beta})\xi_2}$$
$$c_2 = \frac{x(y-x)}{q(y\frac{1-q-\alpha}{\alpha} - x\frac{1-q-\beta}{\beta})\xi_1}$$
$$c_3 = x\frac{x(\frac{1}{q} - \frac{1}{\beta}\frac{1-q-\beta}{\beta}) + y(1-q-\alpha)(\frac{\beta+q}{\beta})}{q(y\frac{1-q-\alpha}{\alpha} - x\frac{1-q-\beta}{\beta})\xi_1}.$$

Using (26), (33) and (34) we find the following expression for the speed of impurity in phase (I):

$$v = \frac{\alpha}{q+\alpha} - (1-q)\rho. \tag{38}$$

One observes that for $\rho > \frac{1-q-\beta}{1-q}$, the average speed of the single impurity again becomes negative. It can easily be checked that in the $q \to 0$ limit the values of ρ_1, ρ_L and v approach to their corresponding values in the phase (VI) of [1]. Next, we will examine the second phase which is characterized with $\xi_2 > \xi_1$. This phase is symmetric to phase (I) and all the results can be obtained using the transformations introduced in section 4. Finally, the third phase (III) occurs when $\xi_1 = \xi_2$, where C is not diagonalizable (see (32)). Nevertheless, Z_L can be computed noting that in this case C can be written as

$$\begin{aligned} C &= \begin{pmatrix} \frac{x}{\beta} + \frac{y}{\alpha} & \frac{x\mathrm{i}}{\sqrt{q}} \\ \frac{\mathrm{i}y}{\sqrt{q}} & x(\frac{\beta+q}{\beta}) + y(\frac{\alpha+q}{\alpha}) \end{pmatrix} \\ &= \left(\frac{x}{\beta} + \frac{y}{\alpha} - x\left(\frac{1-q-\beta}{\beta}\right)\right) I + \begin{pmatrix} x(\frac{1-q-\beta}{\beta}) & \frac{x\mathrm{i}}{\sqrt{q}} \\ \frac{\mathrm{i}y}{\sqrt{q}} & -y(\frac{1-q-\alpha}{\alpha}) \end{pmatrix} \\ &= \left(\frac{x}{\beta} + \frac{y}{\alpha} - x\left(\frac{1-q-\beta}{\beta}\right)\right) I + S \end{aligned} \tag{39}$$

in which

$$S^2 = 0. \tag{40}$$

Using this property with (9) and (29) yields

$$Z_L = \langle W|C^L|V\rangle = \left(x\left(\frac{q+\beta}{\beta}\right) + \frac{y}{\alpha}\right)^{L+1} \left\{x\left(\frac{q+\beta}{\beta}\right) + \frac{y}{\alpha} + Lx\left[\frac{1-q-\beta}{\beta}\right]\right\} \tag{41}$$

and the mean value of density of ordinary particles (22) is found to be

$$\rho = \frac{\sqrt{q}x + \frac{1}{2}(1+q)\sqrt{xy}}{\sqrt{q}x + \sqrt{q}y + (1+q)\sqrt{xy}}. \tag{42}$$

The boundaries of the phase (III) (see figure 3) are limited to

$$\alpha < (1-\rho)(1-q)$$
$$\beta < \rho(1-q)$$

which can be distinguished for $q < 1$ using the fact that $x(\frac{1-q-\beta}{\beta}) = y(\frac{1-q-\alpha}{\alpha})$, (30) and (42). The density profile of ordinary particles, as mentioned above, has an algebraic behaviour in this phase and increases linearly from $\rho_1 = \frac{\beta}{1-q}$ to $\rho_L = 1 - \frac{\alpha}{1-q}$ according to

$$\rho(z) = \frac{\beta}{1-q} + \left(1 - \frac{\beta+\alpha}{1-q}\right) z \qquad 0 \leqslant z \leqslant 1. \tag{43}$$

For $q = 0$, this phase corresponds to phase (V) in [1] where a shock structure has been observed for certain values of the density ρ. The linear profile which is the consequence of a fluctuating shock front, has also been observed in the ASEP and PASEP with open boundaries [11, 15, 16]. Here the relation $x(\frac{1-q-\beta}{\beta}) = y(\frac{1-q-\alpha}{\alpha})$ prevents fixing the fugacities x and y and we cannot adjust the density ρ given by (42) to the desired value, therefore, we cannot see a real shock structure in the grand canonical ensemble. The reason is that relation (22) breaks down in this phase (in the sense that using it one cannot fix the fugacities). As we will show at the end of this section, the density fluctuations of the ordinary particles in this phase, remain finite in the thermodynamic limit. The finiteness of the density fluctuations in open boundary problems predicts the existence of a shock profile. As far as we are using the grand canonical ensemble for this model on a ring, we can also take the finiteness of the fluctuations as a sign for the existance of shock. However, to see a sharp shock profile, one has to go to the canonical ensemble where the density fluctuations disappear in the thermodynamic limit [20]. The speed of impurity (26) in this phase is of the form

$$v = \alpha - \beta \tag{44}$$

which is independent of ρ. Note that for $\beta > \alpha$ the speed of impurity again becomes negative. One can check that in this phase the values of ρ_1, ρ_L and v approach their corresponding values in the phase (V) in $q \to 0$ limit.

The fluctuation in the density of ordinary particles which is given by [18]

$$\left[\frac{x}{L}\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{x}{L}\frac{\mathrm{d}}{\mathrm{d}x}\ln Z_L\right)\right]^{\frac{1}{2}} \tag{45}$$

can also be calculated in each phase. Using (33) one can easily check that, in the large-L limit, these fluctuations drop to zero as $\frac{1}{\sqrt{L}}$ in the phases (I) and (II). Therefore, the results of the grand canonical ensemble agree with those obtained from the canonical one in these phases. It can also be seen from (41) that in phase (III) the fluctuation in the density is finite. This means that the equivalence of the canonical and grand canonical ensemble fails in this phase.

6. Comparison and concluding remarks

As we mentioned in section 2, this model can be considered as a simple generalization of the model studied in [1]. Here we compare the results obtained there (we call it model A) with thoes in our model (model B).

For $q = 0$, the quadratic algebra of model B reduces to the one of model A. Using an infinite-dimensional representation of this algebra, the author has solved model A exactly and shown that it possesses six distinctive phases (I)–(VI). Since we have used a finite-dimensional representation of the quadratic algebra (6)–(8), only the region $\alpha+\beta+q < 1$ lies in the accessible region where three phases exist. These phases (I)–(III) correspond to the phases (VI), (IV) and (V) in model A, respectively. In model A, the density profile of the ordinary particles has an exponential behaviour in phases (VI) and (VI) but has a shock structure in phase (V). In phases (I) and (II) of model B, the density profile also has an exponential behaviour but with a modified correlation length. In region (III) we have obtained a linear profile for the density of the ordinary particles in the grand canonical ensemble which indicates the presence of a shock in this phase. From the phase structure point of view, the backward hopping of the ordinary particles does not change the number of phases at least in the accessible region and only the co-existance lines are shifted.

In this paper we have used a finite-dimensional representation of the algebra and performed all the calculations in the grand canonical ensemble which make the calculations rather simple. It would be interesting to study the region $\alpha + \beta + q > 1$, especially the shock structure in phase (III), using an infinite-dimensional representation of (6)–(8) in the canonical ensemble.

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