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Asymmetric simple exclusion process with open boundaries and Askey–Wilson polynomials

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Abstract
We study the one-dimensional asymmetric simple exclusion process (ASEP) with open boundary conditions. Particles are injected and ejected at both boundaries. It is clarified that the steady state of the model is intimately related to the Askey–Wilson polynomials. The partition function and the n-point functions are obtained in the integral form with four boundary parameters. The thermodynamic current is evaluated to confirm the conjectured phase diagram.

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1. Introduction

In spite of its long history, statistical mechanics for nonequilibrium systems remains to be established. The central principle for the general theory is still lacking. Recently, several analytical and numerical studies of specific nonequilibrium models have revealed their highly interesting behaviour. Among them, exactly solvable models are of great value because physical quantities and their relations are obtained explicitly [1–3].

The one-dimensional asymmetric simple exclusion process (ASEP) is an exactly solvable stochastic process of many particles [3–6]. Particles subject to the exclusion interaction perform random walks with different rates in the right and the left direction. Even after the relaxation to the steady state, the ASEP has nonvanishing particle current, maintained in a nonequilibrium situation. The ASEP has become one of the standard models for the study of nonequilibrium statistical mechanics because of its simplicity, rich behaviour and wide applicability. For instance, the ASEP is regarded as a primitive model of kinetics of biopolymerization [7], traffic flow [8], formation of shocks [9]. It is a discrete version of a hydrodynamic system obeying noisy Burgers equation [10]. It also appears in a kind of sequence alignment problem in computational biology [11].

In this paper we study the ASEP with open boundary conditions. The model has in total five parameters α, β, γ, δ and q. The parameter q is related to the asymmetry of the particle hopping; α (respectively δ) and γ (respectively β) represent the particle input (respectively output) rate at the left and the right boundary respectively. The stationary properties of the model have attracted much attention. Among several reasons, one of them may be that it shows a boundary-induced phase transition [12]; even the bulk properties of the system change drastically depending on the values of the boundary parameters. For the case where particles hop only in one direction ($q = \gamma = \delta = 0$), the current and the density in the thermodynamic limit were calculated in [13, 14]. In [13], the authors introduced a novel algebraic formulation of the problem, which we call the matrix method in the following. This is a method of constructing the exact stationary measure of the model in terms of matrix products. It has become a standard technique for investigating stationary properties of the ASEP and related models. Several generalizations have been considered including discrete time models and multispecies models.

In [13], for the continuous time setting, the algebraic formulation of the solution has been given for the case with the full five parameters although the computation of physical quantities in the thermodynamic limit was performed only for the case where $q = \gamma = \delta = 0$. In [15] the five-parameter case was treated. The current in the thermodynamic limit was calculated and the phase diagram was obtained. The analysis, however, included some approximations. In addition, the computations of other quantities such as the density using the same direction of argument seemed difficult. In [16, 17], the case where $\gamma = \delta = 0$ was studied. The analysis of [16] was based on the findings that the stationary state of the ASEP for the case is related to the q-orthogonal polynomials called the Al-Salam–Chihara polynomials. This method has also admitted the computation of the density profile in [18].

The objective of this paper is to investigate the most general case with the five parameters and further clarify the intimate relationship between the stationary state of the ASEP and the theory of q-orthogonal polynomials. The key is an explicit representation of the matrices and the vectors which realize the stationary state. We will find that the matrix elements coincide with the coefficients which appear in the three-term recurrence relation of the Askey–Wilson polynomials. Then, we exactly calculate the partition function, the n-point functions and other physical quantities. Each quantity is written in an explicit integral form in terms of the moment with respect to the weight function of the Askey–Wilson polynomials. One of the advantages of our approach is that, in our integral representation, the asymptotic behaviour of physical quantities in the thermodynamic limit is easily evaluated using analytical methods for integrals. We can trace the origin of the dominant contribution and how it depends on the boundary parameters. As a result, we confirm the phase diagram for the current obtained in [15].

The paper is organized as follows. In section 2, the definition of the model and physical quantities of the ASEP are introduced. The matrix method is also explained. In section 3, properties of the Askey–Wilson polynomial are reviewed. The recurrence relation and the orthogonality relation play key roles in deriving the integral formula of the partition function. In section 4, two representations of the algebraic relations of matrices are given. One of them is related to the q-Hermite polynomial, which is the special case of the Askey–Wilson polynomial. It is simpler but the parameters are restricted. The other is related to the Askey–Wilson polynomial with full five parameters where no restriction is needed. The connection between the two representations is also mentioned. Section 5 deals with the case where $q = 1$. In section 6, integral formulae of the partition function are derived. In the thermodynamic limit, the asymptotic behaviour of the partition function and bulk quantities of the ASEP are examined. There appears a nonequilibrium phase transition. In section 7, using formulae

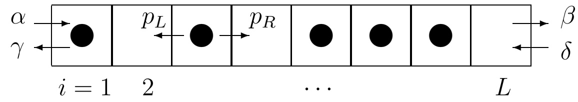

Figure 1. The ASEP with open boundaries.

in the q-calculus, integral formulae of the n-point functions are derived. The last section is devoted to the conclusion.

2. Model and matrix method

The one-dimensional ASEP is a model of randomly hopping particles with exclusion interaction on a one-dimensional lattice [1–6]. Let us denote the system size as L. Each site $i = 1, \ldots, L$ of the lattice can afford at most only one particle; two or more particles cannot remain on the same site due to the hard-core exclusion interaction. A particle hops to the nearest right (respectively left) site with the probability $p_R\,\mathrm{d}t$ (respectively $p_L\,\mathrm{d}t$) during an infinitesimal time $\mathrm{d}t$ if the target site is empty. By rescaling time, we can set $p_R = 1$ and $p_L = q$. In the case of open boundaries, a particle enters the system at the left (respectively right) boundary with rate α (respectively δ) if the site 1 (respectively L) is empty, and is removed at the left (respectively right) boundary with rate γ (respectively β) if the site 1 (respectively L) is occupied. Figure 1 illustrates how the system evolves. Obviously, we can think of the reflection symmetry in this finite system:

$$
\begin{aligned}
&\text{site} \quad i \leftrightarrow L - i + 1 \qquad i = 1, \ldots, L \\
&\text{rate} \quad q \leftrightarrow q^{-1} \qquad \alpha \leftrightarrow q^{-1}\delta \qquad \beta \leftrightarrow q^{-1}\gamma \qquad \gamma \leftrightarrow q^{-1}\beta \qquad \delta \leftrightarrow q^{-1}\alpha.
\end{aligned}
\tag{2.1}
$$

Therefore, the case where $q > 1$ is transformed into the case where $q < 1$ by the symmetry (2.1). In the following, we only assume that the boundary parameters $\alpha, \beta, \gamma, \delta$ are strictly positive unless otherwise stated.

The configuration of the system is labelled by $(\tau_1, \tau_2, \ldots, \tau_L)$ where $\tau_i = 0, 1$ is the particle number at site i. Let $P(\tau_1, \tau_2, \ldots, \tau_L; t)$ denote the probability in the configuration $(\tau_1, \tau_2, \ldots, \tau_L)$ at time t. The time evolution of $P(\tau_1, \tau_2, \ldots, \tau_L; t)$ is described by the master equation,

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} P(\tau_1, \tau_2, \ldots, \tau_L; t) = {}& \delta_{\tau_1,1}[\alpha P(0, \tau_2, \ldots, \tau_L; t) - \gamma P(1, \tau_2, \ldots, \tau_L; t)] \\
& + \delta_{\tau_1,0}[\gamma P(1, \tau_2, \ldots, \tau_L; t) - \alpha P(0, \tau_2, \ldots, \tau_L; t)] \\
& + \sum_{i=1}^{L-1} \big\{ \delta_{(\tau_i,\tau_{i+1})=(1,0)}[q P(\ldots, \tau_i = 0, \tau_{i+1} = 1, \ldots; t) \\
& - P(\ldots, \tau_i = 1, \tau_{i+1} = 0, \ldots; t)] \\
& + \delta_{(\tau_i,\tau_{i+1})=(0,1)}[P(\ldots, \tau_i = 1, \tau_{i+1} = 0, \ldots; t) \\
& - q P(\ldots, \tau_i = 0, \tau_{i+1} = 1, \ldots; t)]\big\} \\
& + \delta_{\tau_L,0}[\beta P(\tau_1, \ldots, \tau_{L-1}, 1; t) - \delta P(\tau_1, \ldots, \tau_{L-1}, 0; t)] \\
& + \delta_{\tau_L,1}[\delta P(\tau_1, \ldots, \tau_{L-1}, 0; t) - \beta P(\tau_1, \ldots, \tau_{L-1}, 1; t)].
\end{aligned}
\tag{2.2}
$$

Hereafter, we focus on the stationary situation of the ASEP. According to the matrix method [13], the stationary solution $P(\tau_1, \tau_2, \ldots, \tau_L)$ for the master equation is obtained in the form,

$$P(\tau_1, \tau_2, \ldots, \tau_L) = \frac{1}{Z_L} \langle W| \prod_{i=1}^{\overrightarrow{L}} (\tau_i \mathsf{D} + (1 - \tau_i)\mathsf{E})|V\rangle. \tag{2.3}$$

Here D and E are matrices; D (respectively E) corresponds to an occupation (respectively emptiness) of a particle. $\langle W|$ and $|V\rangle$ are vectors; $\langle W|$ (respectively $|V\rangle$) corresponds to the left (respectively right) boundary. The normalization constant Z_L is given by

$$Z_L = \langle W|\mathsf{C}^L|V\rangle \tag{2.4}$$

where

$$\mathsf{C} = \mathsf{D} + \mathsf{E}. \tag{2.5}$$

We call Z_L the partition function. One can show that (2.3) gives the exact steady state of the system if the matrices and the vectors satisfy [13]

$$\mathsf{DE} - q\mathsf{ED} = \mathsf{D} + \mathsf{E} \tag{2.6}$$

$$\langle W|(\alpha\mathsf{E} - \gamma\mathsf{D}) = \langle W| \tag{2.7}$$

$$(\beta\mathsf{D} - \delta\mathsf{E})|V\rangle = |V\rangle. \tag{2.8}$$

Physical quantities are written in the form of matrix products. The average particle number at site i, $\langle\tau_i\rangle$, where the bracket means the average over the stationary probability distribution (2.3), is written as

$$\langle\tau_i\rangle = \frac{1}{Z_L}\langle W|\mathsf{C}^{i-1}\mathsf{D}\mathsf{C}^{L-i}|V\rangle \tag{2.9}$$

and the two-point function $\langle\tau_i\tau_j\rangle$ as

$$\langle\tau_i\tau_j\rangle = \frac{1}{Z_L}\langle W|\mathsf{C}^{i-1}\mathsf{D}\mathsf{C}^{j-i-1}\mathsf{D}\mathsf{C}^{L-j}|V\rangle. \tag{2.10}$$

The n-point functions are expressed similarly. The particle current through the bond between the neighbouring sites from left to right, which is defined by $J = \langle\tau_i(1-\tau_{i+1}) - q(1-\tau_i)\tau_{i+1}\rangle$, is simply given by

$$J = \frac{Z_{L-1}}{Z_L}. \tag{2.11}$$

The site dependence of J is unnecessary since the current is uniform for the steady state. One can introduce the fugacity ξ^2 in Z_L as

$$Z_L(\xi^2) = \langle W|(\xi^2\mathsf{D} + \mathsf{E})^L|V\rangle. \tag{2.12}$$

The square of fugacity in the definition is just for convenience. Then, the mean and the variance of the particle density in the whole system are calculated from the first and the second derivatives of $Z_L(\xi^2)$ [19],

$$\langle\rho\rangle = \frac{1}{L}\xi^2\frac{\partial}{\partial\xi^2}\log Z_L(\xi^2)\bigg|_{\xi^2=1} \tag{2.13}$$

$$\langle\Delta\rho^2\rangle = \left(\frac{1}{L}\xi^2\frac{\partial}{\partial\xi^2}\right)^2 \log Z_L(\xi^2)\bigg|_{\xi^2=1}. \tag{2.14}$$

As is familiar in equilibrium statistical physics, the bulk quantities are written in terms of the partition function.

3. Askey–Wilson polynomial

The Askey–Wilson polynomial is a q-orthogonal polynomial with four free parameters besides q. It resides on the top of the hierarchy of the one-variable q-orthogonal polynomial family in the Askey scheme [20–22]. We list several properties of the Askey–Wilson polynomial needed in the following sections. For the purpose we introduce notation heavily used in the q-calculus. In this section, $|q| < 1$ is assumed. The q-shifted factorial:

$$(a_1, a_2, \ldots, a_s; q)_n = \prod_{r=1}^{s} \prod_{k=0}^{n-1} (1 - a_r q^k). \tag{3.1}$$

The basic hypergeometric function:

$${}_r\phi_s \left[\begin{matrix} a_1, \ldots, a_r \\ b_1, \ldots, b_s \end{matrix} ; q, z \right] = \sum_{k=0}^{\infty} \frac{(a_1, \ldots, a_r; q)_k}{(b_1, \ldots, b_s, q; q)_k} ((-1)^k q^{k(k-1)/2})^{1+s-r} z^k. \tag{3.2}$$

Then, the Askey–Wilson polynomial $P_n(x) = P_n(x; a, b, c, d|q)$ is explicitly defined by

$$P_n(x) = a^{-n} (ab, ac, ad; q)_n \, {}_4\phi_3 \left[\begin{matrix} q^{-n}, q^{n-1}abcd, a\,\mathrm{e}^{\mathrm{i}\theta}, a\,\mathrm{e}^{-\mathrm{i}\theta} \\ ab, ac, ad \end{matrix} ; q, q \right] \tag{3.3}$$

with $x = \cos\theta$ for $n \in \mathbb{Z}_+ := \{0, 1, 2, \ldots\}$. It satisfies the three-term recurrence relation,

$$A_n P_{n+1}(x) + B_n P_n(x) + C_n P_{n-1}(x) = 2x P_n(x) \tag{3.4}$$

with $P_0(x) = 1$ and $P_{-1}(x) = 0$, where

$$A_n = \frac{1 - q^{n-1}abcd}{(1 - q^{2n-1}abcd)(1 - q^{2n}abcd)} \tag{3.5}$$

$$B_n = \frac{q^{n-1}}{(1 - q^{2n-2}abcd)(1 - q^{2n}abcd)} \times [(1 + q^{2n-1}abcd)(qs + abcds') - q^{n-1}(1 + q)abcd(s + qs')] \tag{3.6}$$

$$C_n = \frac{(1 - q^n)(1 - q^{n-1}ab)(1 - q^{n-1}ac)(1 - q^{n-1}ad)(1 - q^{n-1}bc)(1 - q^{n-1}bd)(1 - q^{n-1}cd)}{(1 - q^{2n-2}abcd)(1 - q^{2n-1}abcd)} \tag{3.7}$$

and

$$s = a + b + c + d \qquad s' = a^{-1} + b^{-1} + c^{-1} + d^{-1}. \tag{3.8}$$

From this relation, we see that $P_n(x; a, b, c, d|q)$ is symmetric with respect to a, b, c and d. The orthogonality relation depends on the parameter region. If $|a|, |b|, |c|, |d| < 1$, the orthogonality reads

$$\int_0^{\pi} \frac{\mathrm{d}\theta}{2\pi} w(\cos\theta) P_m(\cos\theta) P_n(\cos\theta) = h_n \delta_{mn} \tag{3.9}$$

where

$$w(\cos\theta) = \frac{(\mathrm{e}^{2\mathrm{i}\theta}, \mathrm{e}^{-2\mathrm{i}\theta}; q)_\infty}{(a\,\mathrm{e}^{\mathrm{i}\theta}, a\,\mathrm{e}^{-\mathrm{i}\theta}, b\,\mathrm{e}^{\mathrm{i}\theta}, b\,\mathrm{e}^{-\mathrm{i}\theta}, c\,\mathrm{e}^{\mathrm{i}\theta}, c\,\mathrm{e}^{-\mathrm{i}\theta}, d\,\mathrm{e}^{\mathrm{i}\theta}, d\,\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty} \tag{3.10}$$

$$\frac{h_n}{h_0} = \frac{(1 - q^{n-1}abcd)(q, ab, ac, ad, bc, bd, cd; q)_n}{(1 - q^{2n-1}abcd)(abcd; q)_n} \tag{3.11}$$

$$h_0 = \frac{(abcd; q)_\infty}{(q, ab, ac, ad, bc, bd, cd; q)_\infty}. \tag{3.12}$$

If we rewrite (3.9) with $z = \mathrm{e}^{\mathrm{i}\theta}$, we have

$$\oint_C \frac{\mathrm{d}z}{4\pi \mathrm{i} z} w\left(\frac{z+z^{-1}}{2}\right) P_m\left(\frac{z+z^{-1}}{2}\right) P_n\left(\frac{z+z^{-1}}{2}\right) = h_n \delta_{mn} \tag{3.13}$$

where the integral contour C is a closed path which encloses the poles at $z = aq^k, bq^k, cq^k, \mathrm{d}q^k$ ($k \in \mathbb{Z}_+$) and excludes the poles at $z = (aq^k)^{-1}, (bq^k)^{-1}, (cq^k)^{-1}, (\mathrm{d}q^k)^{-1}$ ($k \in \mathbb{Z}_+$). In other parameter regions, the orthogonality is continued analytically. Putting $m = n = 0$, we have the celebrated Askey–Wilson integral,

$$\oint_C \frac{\mathrm{d}z}{4\pi \mathrm{i} z} \frac{(z^2, z^{-2}; q)_\infty}{(az, a/z, bz, b/z, cz, c/z, dz, d/z; q)_\infty} = \frac{(abcd; q)_\infty}{(q, ab, ac, ad, bc, bd, cd; q)_\infty}. \tag{3.14}$$

For the case of $a = b = c = d = 0$, the Askey–Wilson polynomial is reduced to the q-Hermite polynomial,

$$H_n(x|q) = P_n(x; 0, 0, 0, 0|q). \tag{3.15}$$

Its recurrence and orthogonality relations are those with $a = b = c = d = 0$ in the above formulae for $P_n(x; a, b, c, d|q)$. In what follows, we sometimes write briefly the corresponding weight function or coefficients as $f^{(0)} := f|_{a=b=c=d=0}$. We introduce the q-binomial,

$$F_n(x, y) = \sum_{k=0}^{n} \frac{(q; q)_n}{(q; q)_k (q; q)_{n-k}} x^{n-k} y^k \tag{3.16}$$

which satisfies the following recurrence relation:

$$F_{n+1}(x, y) - (x + y) F_n(x, y) + (1 - q^n) xy F_{n-1}(x, y) = 0 \tag{3.17}$$

with $F_0(x, y) = 1$ and $F_{-1}(x, y) = 0$. The q-Hermite polynomial is a special case of it:

$$H_n(\cos\theta|q) = F_n(\mathrm{e}^{\mathrm{i}\theta}, \mathrm{e}^{-\mathrm{i}\theta}). \tag{3.18}$$

Regarding $F_n(x, y)$, the q-Mehler formula is important:

$$\sum_{n=0}^{\infty} \frac{F_n(v, w) F_n(x, y)}{(q; q)_n} \xi^n = \frac{(vwxy\xi^2; q)_\infty}{(vx\xi, vy\xi, wx\xi, wy\xi; q)_\infty} \tag{3.19}$$

for $|vx\xi|, |vy\xi|, |wx\xi|, |wy\xi| < 1$. Combining (3.17) with this, we obtain another kind of bilinear function:

$$\sum_{n=0}^{\infty} \frac{F_n(v, w) F_{n+1}(x, y)}{(q; q)_n} \xi^n = \frac{x + y - (v + w) xy\xi}{1 - vwxy\xi^2} \frac{(vwxy\xi^2; q)_\infty}{(vx\xi, vy\xi, wx\xi, wy\xi; q)_\infty} \tag{3.20}$$

for $|vx\xi|, |vy\xi|, |wx\xi|, |wy\xi| < 1$.

When $abcd \neq 0$, the symmetry relation for ${}_4\phi_3$,

$${}_4\phi_3\left[\begin{matrix} q^{-n}, a, b, c \\ d, e, f \end{matrix}; q, q\right] = {}_4\phi_3\left[\begin{matrix} q^{n}, a^{-1}, b^{-1}, c^{-1} \\ d^{-1}, e^{-1}, f^{-1} \end{matrix}; q^{-1}, q^{-1}\right] \tag{3.21}$$

implies the symmetry relation for the Askey–Wilson polynomials,

$$P_n(x; a, b, c, d|q) = (-abcd)^n q^{3n(n-1)/2} P_n(x; a^{-1}, b^{-1}, c^{-1}, d^{-1}|q^{-1}). \tag{3.22}$$

From this symmetry, it is enough to study the case where $|q| < 1$. But when $abcd = 0$, this relation no longer holds and one has to consider the case where $q > 1$ separately [23, 24]. For instance, suppose that only one of a, b, c, d is zero. Without loss of generality, we can set

$d = 0$ because of the symmetry in a, b, c, d. The recurrence relation (3.4) remains the same (with d set to zero), but the orthogonality relation (3.9) should be modified. $P_n(x)$ are now orthogonal on the imaginary axis;

$$\int_{-\infty}^{\infty} \mathrm{d}u\, \widetilde{w}(\sinh u) P_m(\mathrm{i}\sinh u) P_n(\mathrm{i}\sinh u) = \widetilde{h}_n \delta_{mn} \tag{3.23}$$

where

$$\widetilde{w}(\sinh u) = \frac{1}{\log q} \frac{(\mathrm{i}aq^{-1}\,\mathrm{e}^{u}, -\mathrm{i}aq^{-1}\,\mathrm{e}^{-u}, \mathrm{i}bq^{-1}\,\mathrm{e}^{u}, -\mathrm{i}bq^{-1}\,\mathrm{e}^{-u}, \mathrm{i}cq^{-1}\,\mathrm{e}^{u}, -\mathrm{i}cq^{-1}\,\mathrm{e}^{-u}; q^{-1})_\infty}{(-q^{-1}\,\mathrm{e}^{2u}, -q^{-1}\,\mathrm{e}^{-2u}; q^{-1})_\infty} \tag{3.24}$$

$$\widetilde{h}_n = (q, ab, ac, bc; q)_n (q^{-1}, abq^{-1}, acq^{-1}, bcq^{-1}; q^{-1})_\infty. \tag{3.25}$$

The formulae when more than one of a, b, c, d are zero are similar. For details about the case where $q > 1$, we refer the reader to [23, 24]. The list of formulae exploited in the following sections is completed.

4. Representation: the case where $q \neq 1$

In the subsequent sections we give two infinite-dimensional representations of matrices and vectors. One is related to the q-Hermite polynomials and the other to the Askey–Wilson polynomials. The representations are useful since the q-orthogonal polynomial forms a complete set of eigenvectors of the matrix C, which enters the matrix expression of Z_L (2.4). In the following the parameters are fixed as

$$a = \kappa^+_{\alpha,\gamma} \qquad b = \kappa^+_{\beta,\delta} \qquad c = \kappa^-_{\alpha,\gamma} \qquad d = \kappa^-_{\beta,\delta} \tag{4.1}$$

where

$$\kappa^{\pm}_{\alpha,\gamma} = \frac{1}{2\alpha}\left[(1 - q - \alpha + \gamma) \pm \sqrt{(1 - q - \alpha + \gamma)^2 + 4\alpha\gamma}\right] \tag{4.2}$$

$$\kappa^{\pm}_{\beta,\delta} = \frac{1}{2\beta}\left[(1 - q - \beta + \delta) \pm \sqrt{(1 - q - \beta + \delta)^2 + 4\beta\delta}\right]. \tag{4.3}$$

We also fix q as $0 < q < 1$; the $q > 1$ case is simply considered from the reflection symmetry (2.1), or equivalently,

$$a, b, c, d, q \leftrightarrow b^{-1}, a^{-1}, d^{-1}, c^{-1}, q^{-1}. \tag{4.4}$$

Since $\alpha, \beta, \gamma, \delta$ are strictly positive, the new parameters satisfy $a > 0, b > 0, -1 < c < 0$ and $-1 < d < 0$ if $0 < q < 1$. The bra and ket notations are used for row and column vectors, respectively. In place of matrices D and E, we consider d and e,

$$\mathsf{D} = \frac{1}{1-q}(1 + \mathsf{d}) \qquad \mathsf{E} = \frac{1}{1-q}(1 + \mathsf{e}) \tag{4.5}$$

$$\mathsf{C} = \mathsf{D} + \mathsf{E} = \frac{1}{1-q}(21 + \mathsf{d} + \mathsf{e}). \tag{4.6}$$

For these matrices the relations (2.6), (2.7) and (2.8) are replaced by

$$\mathsf{de} - q\mathsf{ed} = (1-q)\mathsf{1} \tag{4.7}$$

$$\langle W|[\mathsf{e} - (a+c)\mathsf{1} + ac\mathsf{d}] = 0 \tag{4.8}$$

$$[\mathsf{d} - (b+d)\mathsf{1} + bd\mathsf{e}]|V\rangle = 0. \tag{4.9}$$

4.1. Representation related to the q-Hermite polynomials

First, we give a representation related to the q-Hermite polynomials. One can check that the following matrices and vectors satisfy the relations (4.7), (4.8) and (4.9).

$$\mathsf{d} = \begin{bmatrix} 0 & \sqrt{1-q} & 0 & \cdots \\ 0 & 0 & \sqrt{1-q^2} & \\ 0 & 0 & 0 & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \qquad \mathsf{e} = \begin{bmatrix} 0 & 0 & 0 & \cdots \\ \sqrt{1-q} & 0 & 0 & \\ 0 & \sqrt{1-q^2} & 0 & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \tag{4.10}$$

$$\begin{aligned} \langle W| &= \nu_{a,c}\big(F_0(a,c)\big/\sqrt{(q;q)_0},\, F_1(a,c)\big/\sqrt{(q;q)_1},\ldots\big) \\ |V\rangle &= \nu_{b,d}\big(F_0(b,d)\big/\sqrt{(q;q)_0},\, F_1(b,d)\big/\sqrt{(q;q)_1},\ldots\big)^T \end{aligned} \tag{4.11}$$

where $\nu_{a,c} = (ac;q)_\infty^{-1}(q;q)_\infty^{-1/2}$. We regard (4.7) as the q-deformed commutation relation of boson operators [25–27], and (4.10) and (4.11) as the q-deformed Fock representation [17]. Note that matrices d and e depend only on q, and vectors $\langle W|$ and $|V\rangle$ depend on q and the boundary parameters. In this representation, a vector defined by

$$|h(x)\rangle = (h_0(x), h_1(x), h_2(x), \ldots)^T \tag{4.12}$$

where

$$h_n(x) = \sqrt{\frac{(q;q)_\infty}{(q;q)_n}}\, H_n(x|q) \tag{4.13}$$

is eigenvector of the matrix $\mathsf{d}+\mathsf{e}$ with the eigenvalue $2x$:

$$(\mathsf{d}+\mathsf{e})|h(x)\rangle = 2x|h(x)\rangle. \tag{4.14}$$

Each element of this equation corresponds to the recurrence relation of the q-Hermite polynomials. The transposed equation also holds for $\langle h(x)| := |h(x)\rangle^T$ because $\mathsf{d}+\mathsf{e}$ is a symmetric matrix. The orthogonality relation is rewritten as

$$\mathsf{1} = \int_0^\pi \frac{\mathrm{d}\theta}{2\pi} w^{(0)}(\cos\theta)|h(\cos\theta)\rangle\langle h(\cos\theta)|. \tag{4.15}$$

Therefore, the eigenvector of $\mathsf{d}+\mathsf{e}$, or at the same time the eigenvector of C from (4.6), $\{|h(\cos\theta)\rangle; \theta \in [0,\pi]\}$ forms a complete set of vectors in this representation space. Furthermore, from (3.20) with (3.18) we obtain the following form factor:

$$\langle h(\cos\theta)|\Lambda(\xi)\mathsf{d}|h(\cos\phi)\rangle = \frac{(q,\xi^2 q;q)_\infty(2\cos\phi - 2\xi\cos\theta)}{(\xi\,\mathrm{e}^{\mathrm{i}(\theta+\phi)}, \xi\,\mathrm{e}^{-\mathrm{i}(\theta+\phi)}, \xi\,\mathrm{e}^{\mathrm{i}(\theta-\phi)}, \xi\,\mathrm{e}^{-\mathrm{i}(\theta-\phi)};q)_\infty}. \tag{4.16}$$

Here a regularization matrix $\Lambda(\xi) = \mathrm{diag}(1,\xi,\xi^2,\ldots)$ is introduced.

In fact, this representation is valid only when $|a|, |b|, |c|, |d| < 1$, otherwise, the boundary vectors are ill-defined. For example, if $a > 1$, $\langle W|h(\cos\theta)\rangle$ becomes a divergent series. See the convergence condition for the q-Mehler formula (3.19). In the next subsection, we present another representation without such restriction.

4.2. Representation related to the Askey–Wilson polynomial

We consider a representation related to the Askey–Wilson polynomials with full five parameters. Here a, b, c, d are not restricted. Apparently complicated, the following equations certainly solve equations (4.7), (4.8) and (4.9):

$$\mathsf{d} = \begin{bmatrix} d_0^\natural & d_0^\sharp & 0 & \cdots \\ d_0^\flat & d_1^\natural & d_1^\sharp & \\ 0 & d_1^\flat & d_2^\natural & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \qquad \mathsf{e} = \begin{bmatrix} e_0^\natural & e_0^\sharp & 0 & \cdots \\ e_0^\flat & e_1^\natural & e_1^\sharp & \\ 0 & e_1^\flat & e_2^\natural & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \tag{4.17}$$

$$\langle W| = h_0^{1/2}(1, 0, 0, \ldots) \qquad |V\rangle = h_0^{1/2}(1, 0, 0, \ldots)^T \tag{4.18}$$

where

$$\begin{aligned} d_n^\natural = \frac{q^{n-1}}{(1-q^{2n-2}abcd)(1-q^{2n}abcd)}[&bd(a+c) + (b+d)q - abcd(b+d)q^{n-1} \\ &- \{bd(a+c) + abcd(b+d)\}q^n - bd(a+c)q^{n+1} \\ &+ ab^2cd^2(a+c)q^{2n-1} + abcd(b+d)q^{2n}] \end{aligned} \tag{4.19}$$

$$\begin{aligned} e_n^\natural = \frac{q^{n-1}}{(1-q^{2n-2}abcd)(1-q^{2n}abcd)}[&ac(b+d) + (a+c)q - abcd(a+c)q^{n-1} \\ &- \{ac(b+d) + abcd(a+c)\}q^n - ac(b+d)q^{n+1} \\ &+ a^2bc^2d(b+d)q^{2n-1} + abcd(a+c)q^{2n}] \end{aligned} \tag{4.20}$$

$$d_n^\sharp = \frac{1}{1-q^n ac}\mathcal{A}_n \qquad e_n^\sharp = -\frac{q^n ac}{1-q^n ac}\mathcal{A}_n \tag{4.21}$$

$$d_n^\flat = -\frac{q^n bd}{1-q^n bd}\mathcal{A}_n \qquad e_n^\flat = \frac{1}{1-q^n bd}\mathcal{A}_n \tag{4.22}$$

and

$$\begin{aligned} \mathcal{A}_n = [\{&(1-q^{n-1}abcd)(1-q^{n+1})(1-q^n ab)(1-q^n ac)(1-q^n ad)(1-q^n bc)(1-q^n bd) \\ &\times(1-q^n cd)\}/\{(1-q^{2n-1}abcd)(1-q^{2n}abcd)^2(1-q^{2n+1}abcd)\}]^{1/2}. \end{aligned} \tag{4.23}$$

As before, a vector defined by

$$|p(x)\rangle = (p_0(x), p_1(x), p_2(x), \ldots)^T \tag{4.24}$$

where

$$p_n(x) = \sqrt{\frac{h_0}{h_n}} P_n(x; a, b, c, d|q) \tag{4.25}$$

becomes the eigenvector of the matrix $\mathsf{d} + \mathsf{e}$ with the eigenvalue $2x$:

$$(\mathsf{d} + \mathsf{e})|p(x)\rangle = 2x|p(x)\rangle. \tag{4.26}$$

Each element of this equation corresponds to the recurrence relation of the Askey–Wilson polynomials (3.4). The transposed equation also holds for $\langle p(x)| := |p(x)\rangle^T$ because $\mathsf{d}+\mathsf{e}$ is a symmetric matrix. The orthogonality relation (3.9) is rewritten as

$$\mathsf{1} = h_0^{-1} \oint_C \frac{\mathrm{d}z}{4\pi \mathrm{i} z} w((z+z^{-1})/2)|p((z+z^{-1})/2)\rangle\langle p((z+z^{-1})/2)| \tag{4.27}$$

where the contour C is as described below (3.13). The reflection (4.4) corresponds to just taking transpositions in the representation. If we set $c = d = 0$, or equivalently $\gamma = \delta = 0$, we find that the representation is reduced to the one related to the Al-Salam–Chihara polynomials [16].

The relation between the representation here and the previous one is almost obvious. They are equivalent if $|a|, |b|, |c|, |d| < 1$. The connection matrix comes from the transformation,

$$\frac{h_0^{-1/2}}{(a\,\mathrm{e}^{\mathrm{i}\theta}, a\,\mathrm{e}^{-\mathrm{i}\theta}, c\,\mathrm{e}^{\mathrm{i}\theta}, c\,\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}|p(\cos\theta)\rangle = G^{(a,c)}_{(b,d)}|h(\cos\theta)\rangle. \tag{4.28}$$

We can calculate the elements as

$$\left[G^{(a,c)}_{(b,d)}\right]_{n,k} = \frac{(ab, ac, ad; q)_n}{a^n (ac; q)_\infty \sqrt{h_n (q; q)_k (q; q)_\infty}} \sum_{j=0}^{n} \frac{(q^{-n}, q^{n-1}abcd; q)_j q^j}{(q, ab, ad; q)_j} F_k(aq^j, c). \tag{4.29}$$

The inverse matrix is given by

$$\left[G^{(a,c)}_{(b,d)}\right]^{-1} = \left[G^{(b,d)}_{(a,c)}\right]^T. \tag{4.30}$$

To prove this, compare the two orthogonality relations (4.15) and (4.27). Replacing $(a, c) \leftrightarrow (b, d)$ and transposing in (4.28), we have

$$\frac{h_0^{-1/2}}{(b\,\mathrm{e}^{\mathrm{i}\theta}, b\,\mathrm{e}^{-\mathrm{i}\theta}, d\,\mathrm{e}^{\mathrm{i}\theta}, d\,\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}\langle p(\cos\theta)| = \langle h(\cos\theta)|\left[G^{(b,d)}_{(a,c)}\right]^T. \tag{4.31}$$

Then,

$$\begin{aligned}
\mathsf{1} &= h_0^{-1} \int_0^\pi \frac{\mathrm{d}\theta}{2\pi} w(\cos\theta)|p(\cos\theta)\rangle\langle p(\cos\theta)| \\
&= \int_0^\pi \frac{\mathrm{d}\theta}{2\pi} w^{(0)}(\cos\theta) G^{(a,c)}_{(b,d)}|h(\cos\theta)\rangle\langle h(\cos\theta)|\left[G^{(b,d)}_{(a,c)}\right]^T \\
&= G^{(a,c)}_{(b,d)}\left[G^{(b,d)}_{(a,c)}\right]^T.
\end{aligned}$$

This matrix actually connects the two representations since, for example, $\langle W|^{\mathrm{Hermite}} = \langle W|^{\mathrm{AW}} G^{(a,c)}_{(b,d)}$.

Looking at the form factor in the q-Hermite representation (4.16), a nontrivial formula results in the Askey–Wilson representation;

$$\begin{aligned}
&\langle p(\cos\theta)|\Theta(\xi)\mathsf{d}|p(\cos\phi)\rangle \\
&= \frac{(2\cos\phi - 2\xi\cos\theta)(q, \xi^2 q, a\,\mathrm{e}^{\mathrm{i}\phi}, a\,\mathrm{e}^{-\mathrm{i}\phi}, c\,\mathrm{e}^{\mathrm{i}\phi}, c\,\mathrm{e}^{-\mathrm{i}\phi}, b\,\mathrm{e}^{\mathrm{i}\theta}, b\,\mathrm{e}^{-\mathrm{i}\theta}, d\,\mathrm{e}^{\mathrm{i}\theta}, d\,\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}{(\xi\,\mathrm{e}^{\mathrm{i}(\theta+\phi)}, \xi\,\mathrm{e}^{\mathrm{i}(\theta-\phi)}, \xi\,\mathrm{e}^{-\mathrm{i}(\theta+\phi)}, \xi\,\mathrm{e}^{-\mathrm{i}(\theta-\phi)}; q)_\infty}
\end{aligned} \tag{4.32}$$

where

$$\Theta(\xi) = G^{(a,c)}_{(b,d)}\Lambda(\xi)\left[G^{(a,c)}_{(b,d)}\right]^{-1}. \tag{4.33}$$

The matrix elements are explicitly calculated as

$$
\begin{aligned}
[\Theta(\xi)]_{n,k} = \frac{1}{\sqrt{h_n h_k}} & \frac{(abcd\xi^2;q)_\infty (ab,ac,ad;q)_n (ab,bc,bd;q)_k}{(q,ab\xi,ac,ad\xi,bc\xi,bd,cd\xi;q)_\infty} a^{-n} b^{-k} \\
& \times \sum_{j=0}^{n} \frac{(q^{-n},q^{n-1}abcd,ab\xi,ad\xi;q)_j q^j}{(q,ab,ad,abcd\xi^2;q)_j} \\
& \times {}_4\phi_3 \left[\begin{matrix} q^{-k},q^{k-1}abcd,ab\xi q^j,bc\xi \\ ab,bc,abcd\xi q^j \end{matrix} ;q,q \right].
\end{aligned} \tag{4.34}
$$

A remark on a special case is in order. When we specialize to the case where $ab = q^{1-N}$ $(N = 1,2,\ldots)$, the infinite-dimensional representation can be reduced to an N-dimensional one. The same is true for other pairwise products of a,b,c,d because of the symmetry in a,b,c,d. The matrices can be taken from the first $N \times N$ entries of those of the infinite-dimensional matrices, and similarly the first N entries for the vectors:

$$
\mathsf{d}^{(N)} = \begin{bmatrix} d_0^\natural & d_0^\sharp & 0 & \cdots \\ d_0^\flat & d_1^\natural & \ddots & \\ 0 & \ddots & \ddots & d_{N-2}^\sharp \\ \vdots & & d_{N-2}^\flat & d_{N-1}^\natural \end{bmatrix} \qquad \mathsf{e}^{(N)} = \begin{bmatrix} e_0^\natural & e_0^\sharp & 0 & \cdots \\ e_0^\flat & e_1^\natural & \ddots & \\ 0 & \ddots & \ddots & e_{N-2}^\sharp \\ \vdots & & e_{N-2}^\flat & e_{N-1}^\natural \end{bmatrix} \tag{4.35}
$$

$$
\langle W^{(N)}| = h_0^{1/2}(1,0,\ldots,0) \qquad |V^{(N)}\rangle = h_0^{1/2}(1,0,\ldots,0)^T. \tag{4.36}
$$

In this case, the corresponding Askey–Wilson polynomials are called the q-Racah polynomials. The orthogonality relation is rewritten in N residue sum from the integral form. This special case may be useful for trial calculations of many quantities of the ASEP since a generally difficult task of integration is replaced by finite summation. In fact, this finite-dimensional representation is equivalent to the one in [28, 29]. The similarity transformation is realized by an $N \times N$ matrix U:

$$
U_{nk} = \frac{(ab,ac,ad;q)_n (ab,bc;q)_k}{a^n(-b)^k q^{k(k-1)/2}\sqrt{h_n}} {}_3\phi_2 \left[\begin{matrix} q^{-n},q^{n-1}abcd,abq^k \\ ab,ad \end{matrix} ;q,q \right] \tag{4.37}
$$

for $n,k = 0,\ldots,N-1$. Then,

$$
U^{-1}\mathsf{d}^{(N)}U = \begin{bmatrix} b & 0 & 0 & \cdots & \cdots \\ 0 & bq & \ddots & & \\ 0 & 0 & bq^2 & \ddots & \\ \vdots & & \ddots & \ddots & 0 \\ & & & 0 & bq^{N-1} \end{bmatrix} \tag{4.38}
$$

$$
U^{-1}\mathsf{e}^{(N)}U = \begin{bmatrix} b^{-1} & 0 & 0 & \cdots & \cdots \\ 1 & (bq)^{-1} & \ddots & & \\ 0 & 1 & (bq^2)^{-1} & \ddots & \\ \vdots & & \ddots & \ddots & 0 \\ & & & 1 & (bq^{N-1})^{-1} \end{bmatrix} \tag{4.39}
$$

$$\langle W^{(N)}|U = (1, U_{01}, \ldots, U_{0,N-1}) \tag{4.40}$$

$$U^{-1}|V^{(N)}\rangle = ((U^{-1})_{00}, (U^{-1})_{10}, \ldots, (U^{-1})_{N-1,0})^T. \tag{4.41}$$

5. Representation: the case where $q = 1$

In this section a representation for $q = 1$ is given. We consider matrices D and E instead of d and e. Taking the limit $q \to 1$ in the representation in section 4.2 yields

$$\mathsf{D} = \begin{bmatrix} D_0^\natural & D_0^\sharp & 0 & \cdots \\ D_0^\flat & D_1^\natural & D_1^\sharp & \\ 0 & D_1^\flat & D_2^\natural & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \qquad \mathsf{E} = \begin{bmatrix} E_0^\natural & E_0^\sharp & 0 & \cdots \\ E_0^\flat & E_1^\natural & E_1^\sharp & \\ 0 & E_1^\flat & E_2^\natural & \ddots \\ \vdots & & \ddots & \ddots \end{bmatrix} \tag{5.1}$$

$$\langle W| = (1, 0, 0, \ldots) \qquad |V\rangle = (1, 0, 0, \ldots)^T \tag{5.2}$$

where

$$\begin{aligned} D_n^\natural &= \frac{\alpha + \delta + n(\alpha\beta + 2\alpha\delta + \gamma\delta)}{(\alpha+\gamma)(\beta+\delta)} & E_n^\natural &= \frac{\beta + \gamma + n(\alpha\beta + 2\beta\gamma + \gamma\delta)}{(\alpha+\gamma)(\beta+\delta)} \\ D_n^\sharp &= \frac{\alpha}{\alpha+\gamma}[(n+1)(\lambda+n+1)]^{1/2} & E_n^\sharp &= \frac{\gamma}{\alpha+\gamma}[(n+1)(\lambda+n+1)]^{1/2} \\ D_n^\flat &= \frac{\delta}{\beta+\delta}[(n+1)(\lambda+n+1)]^{1/2} & E_n^\flat &= \frac{\beta}{\beta+\delta}[(n+1)(\lambda+n+1)]^{1/2} \end{aligned} \tag{5.3}$$

with

$$\lambda = \frac{\alpha+\beta+\gamma+\delta}{(\alpha+\gamma)(\beta+\delta)} - 1. \tag{5.4}$$

The eigenvector of C is

$$|\ell(x)\rangle = (\ell_0(x), \ell_1(x), \ldots)^T \tag{5.5}$$

where the elements are

$$\ell_n(x) = (-1)^n \left[\frac{n!\Gamma(\lambda+1)}{\Gamma(\lambda+n+1)}\right]^{1/2} L_n^{(\lambda)}(x). \tag{5.6}$$

The orthogonal polynomials in this case are the Laguerre polynomials $L_n^{(\lambda)}(x)$. The recurrence relation of $L_n^{(\lambda)}(x)$ is

$$(n+1)L_{n+1}^{(\lambda)}(x) - (2n+\lambda+1-x)L_n^{(\lambda)}(x) + (n+\lambda)L_{n-1}^{(\lambda)}(x) = 0 \tag{5.7}$$

with $L_0^{(\lambda)}(x) = 1$ and $L_{-1}^{(\lambda)}(x) = 0$. In our notation it is rewritten as

$$\mathsf{C}|\ell(x)\rangle = x|\ell(x)\rangle. \tag{5.8}$$

The orthogonality relation reads

$$\int_0^\infty \mathrm{d}x\, x^\lambda\, \mathrm{e}^{-x} L_m^{(\lambda)}(x) L_n^{(\lambda)}(x) = \frac{\Gamma(n+\lambda+1)}{n!}\delta_{mn} \tag{5.9}$$

for $\lambda > -1$. It is rewritten as

$$1 = \mu^{-1}\int_0^\infty \mathrm{d}x\, x^\lambda\, \mathrm{e}^{-x} |\ell(x)\rangle\langle\ell(x)| \tag{5.10}$$

where $\mu = \Gamma(\lambda + 1)$. We can obtain the form factor as

$$\langle \ell(x)|\mathsf{D}|\ell(y)\rangle = \mu^{-1}\left[(c_1 + c_2 x)x^{-\lambda}\,\mathrm{e}^x\delta(y - x) + c_3 \lim_{z\to 1}\mathcal{J}(x, y, z)\right] \tag{5.11}$$

where

$$c_1 = -\frac{\alpha\beta - \gamma\delta}{(\alpha + \gamma)^2(\beta + \delta)} \qquad c_2 = \frac{\alpha}{\alpha + \gamma} \qquad c_3 = -\frac{\alpha\beta - \gamma\delta}{(\alpha + \gamma)(\beta + \delta)} \tag{5.12}$$

$$\mathcal{J}(x, y, z) = \frac{1}{1 - z}[xyz\mathcal{I}_{\lambda+1}(x, y, z) - yz\mathcal{I}_\lambda(x, y, z)] \tag{5.13}$$

$$\begin{aligned}\mathcal{I}_\lambda(x, y, z) &= \sum_{n=0}^{\infty}\frac{n!}{\Gamma(n + \lambda + 1)}L_n^{(\lambda)}(x)L_n^{(\lambda)}(y)z^n \\ &= \frac{(xyz)^{-\lambda/2}}{1 - z}\exp\left(-\frac{(x + y)z}{1 - z}\right)I_\lambda\left(\frac{2(xyz)^{1/2}}{1 - z}\right).\end{aligned} \tag{5.14}$$

Here $I_\lambda(z)$ is the modified Bessel function.

6. Partition function Z_L and bulk quantities

Applying the formulae presented in the previous sections, the partition functions of the ASEP, Z_L, are obtained in the integral form. Bulk quantities are obtained through the partition function. The results are of course independent of the choice of representation.

6.1. The case where $q \neq 1$

We consider the representation in section 4.2 since the boundary parameters are unrestricted. First, consider the $q < 1$ case. Inserting the identity operator (4.27) in (2.4), we have

$$\begin{aligned}Z_L &= \langle W|\mathsf{C}^L|V\rangle \\ &= h_0^{-1}\oint_C \frac{\mathrm{d}z}{4\pi\mathrm{i}z}w((z + z^{-1})/2)\langle W|p((z + z^{-1})/2)\rangle\langle p((z + z^{-1})/2)|\mathsf{C}^L|V\rangle \\ &= h_0^{-1}\oint_C \frac{\mathrm{d}z}{4\pi\mathrm{i}z}w\langle W|p((z + z^{-1})/2)\rangle\langle p((z + z^{-1})/2)|V\rangle\left[\frac{(1 + z)(1 + z^{-1})}{1 - q}\right]^L \\ &= \oint_C \frac{\mathrm{d}z}{4\pi\mathrm{i}z}w((z + z^{-1})/2)\left[\frac{(1 + z)(1 + z^{-1})}{1 - q}\right]^L.\end{aligned}$$

In the third line, we used (4.26). The integral formula of the partition function is now obtained:

$$Z_L = \oint_C \frac{\mathrm{d}z}{4\pi\mathrm{i}z}\frac{(z^2, z^{-2}; q)_\infty[(1 + z)(1 + z^{-1})/(1 - q)]^L}{(az, a/z, bz, b/z, cz, c/z, dz, d/z; q)_\infty} \tag{6.1}$$

where the integral contour C is a closed path which encloses the poles at $z = aq^k, bq^k, cq^k, dq^k$ $(k \in \mathbb{Z}_+)$ and excludes the poles at $z = (aq^k)^{-1}, (bq^k)^{-1}, (cq^k)^{-1}, (dq^k)^{-1}$ $(k \in \mathbb{Z}_+)$. The partition function with the fugacity (2.12) is similarly obtained with replacements $a \to a\xi^{-1}, b \to b\xi, c \to c\xi^{-1}, d \to d\xi$:

$$Z_L(\xi^2) = \oint_C \frac{\mathrm{d}z}{4\pi\mathrm{i}z}\frac{(z^2, z^{-2}; q)_\infty[(1 + \xi z)(1 + \xi z^{-1})/(1 - q)]^L}{(a\xi^{-1}z, a\xi^{-1}/z, b\xi z, b\xi/z, c\xi^{-1}z, c\xi^{-1}/z, d\xi z, d\xi/z; q)_\infty}. \tag{6.2}$$

The partition functions finally have the form of the moment integral with respect to the weight function of the Askey–Wilson polynomials. The result is independent of our approach;

however, it should be noted that the origin of the weight function and the role of the Askey–Wilson polynomials have become transparent through the finding of the explicit representation of the matrices in the matrix method.

These integrals have the same compact form for all values of the parameters. Below, we examine detailed cases and confirm the drastic dependence on the boundary parameters. The integral is difficult to evaluate, but its asymptotic behaviour in the thermodynamic limit $L \gg 1$ is obtained without difficulty. We should consider three cases: (A) $a > 1$ and $a > b$, (B) $b > 1$ and $b > a$ and (C) $a < 1$ and $b < 1$.

(A) $a > 1$ and $a > b$: In the integral, the dominant contribution comes from the residue of the poles at $z = a, a^{-1}$ of order $[(1+a)(1+a^{-1})/(1-q)]^L$. Therefore, we have an approximation of Z_L as

$$Z_L^{(a)} \simeq \frac{(a^{-2};q)_\infty}{(q, ab, ac, ad, a^{-1}b, a^{-1}c, a^{-1}d; q)_\infty}\left[\frac{(1+a)(1+a^{-1})}{1-q}\right]^L. \tag{6.3}$$

Similarly, for the partition function with fugacity, we have

$$Z_L^{(a)}(\xi^2) \simeq \frac{(a^{-2}\xi^2;q)_\infty}{(q, ab, ac\xi^{-2}, ad, a^{-1}b\xi^2, a^{-1}c, a^{-1}d\xi^2; q)_\infty}\left[\frac{(1+a)(1+a^{-1}\xi^2)}{1-q}\right]^L. \tag{6.4}$$

Then, the bulk quantities (2.11), (2.13) and (2.14) are calculated as

$$J \simeq (1-q)\frac{a}{(1+a)^2} \qquad \langle\rho\rangle \simeq \frac{1}{1+a} \qquad \langle\Delta\rho^2\rangle \simeq \frac{a}{(1+a)^2 L}. \tag{6.5}$$

(B) $b > 1$ and $b > a$: The results are similarly obtained as (A):

$$Z_L^{(b)} \simeq \frac{(b^{-2};q)_\infty}{(q, ba, bc, bd, b^{-1}a, b^{-1}c, b^{-1}d; q)_\infty}\left[\frac{(1+b)(1+b^{-1})}{1-q}\right]^L. \tag{6.6}$$

$$Z_L^{(b)}(\xi^2) \simeq \frac{(b^{-2}\xi^{-2};q)_\infty}{(q, ba, bc, bd\xi^2, b^{-1}a\xi^{-2}, b^{-1}c\xi^{-2}, b^{-1}d; q)_\infty}\left[\frac{(1+b\xi^2)(1+b^{-1})}{1-q}\right]^L. \tag{6.7}$$

Then, we have

$$J \simeq (1-q)\frac{b}{(1+b)^2} \qquad \langle\rho\rangle \simeq \frac{b}{1+b} \qquad \langle\Delta\rho^2\rangle \simeq \frac{b}{(1+b)^2 L}. \tag{6.8}$$

(C) $a < 1$ and $b < 1$: The contour integral is just over a unit circle and can be approximated around $z = 1$ by the steepest descent method:

$$Z_L^{(0)} \simeq \frac{(q;q)_\infty^2}{(a,b,c,d;q)_\infty^2}\frac{4}{\sqrt{\pi}L^{3/2}}\left(\frac{4}{1-q}\right)^L. \tag{6.9}$$

$$Z_L^{(0)}(\xi^2) \simeq \frac{(q;q)_\infty^2}{(a\xi^{-1}, b\xi, c\xi^{-1}, d\xi;q)_\infty^2}\frac{[(1+\xi)(1+\xi^{-1})]^{3/2}}{2\sqrt{\pi}L^{3/2}}\left[\frac{(1+\xi)^2}{1-q}\right]^L. \tag{6.10}$$

Then, we have

$$J \simeq \frac{1-q}{4} \qquad \langle\rho\rangle \simeq \frac{1}{2} \qquad \langle\Delta\rho^2\rangle \simeq \frac{1}{8L}. \tag{6.11}$$

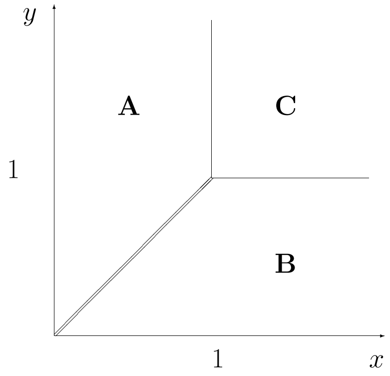

Figure 2. The phase diagram of the ASEP. There are three phases; phase A: low-density phase, phase B: high-density phase and phase C: maximal-current phase. $(x, y) = (a^{-1}, b^{-1})$ if $q < 1$, and $(x, y) = (b, a)$ if $q > 1$. a and b are defined in (4.1). The double line is for a transition of first order and the solid line is for that of second order.

The results for $q > 1$ are directly from the above expressions considering the reflection symmetry (4.4).

(A′) $b^{-1} > 1$ and $b^{-1} > a^{-1}$:

$$J \simeq -(1-q^{-1})\frac{b}{(1+b)^2} \qquad \langle\rho\rangle \simeq \frac{b}{1+b} \qquad \langle\Delta\rho^2\rangle \simeq \frac{b}{(1+b)^2 L}. \tag{6.12}$$

(B′) $a^{-1} > 1$ and $a^{-1} > b^{-1}$:

$$J \simeq -(1-q^{-1})\frac{a}{(1+a)^2} \qquad \langle\rho\rangle \simeq \frac{1}{1+a} \qquad \langle\Delta\rho^2\rangle \simeq \frac{a}{(1+a)^2 L}. \tag{6.13}$$

(C′) $a^{-1} < 1$ and $b^{-1} < 1$:

$$J \simeq -\frac{1-q^{-1}}{4} \qquad \langle\rho\rangle \simeq \frac{1}{2} \qquad \langle\Delta\rho^2\rangle \simeq \frac{1}{8L}. \tag{6.14}$$

The minus sign in the front of the current is due to the parity change under the reflection.

In this way, we have three phases altogether. The phase A is called the low-density phase, the phase B the high-density phase and the phase C the maximal-current phase. In fact, the average of the particle density increases in the order phase A, phase C, phase B. The particle current takes the maximum value in phase C. Figure 2 shows the phase diagram of J and $\langle\rho\rangle$. The same diagram as that in [15] is reproduced. It is remarkable that the phases are determined by the dominant contribution from a few points of the integral of the partition function and we can note that they are replaced by one another depending on the boundary parameters. We can refer to the order of the phase transitions. We observe that across the line between the phases A and B, the first derivative of J is discontinuous and $\langle\rho\rangle$ itself is discontinuous. Across the lines between phases A and C, or phases B and C, the second derivative of J is discontinuous and the first derivative of $\langle\rho\rangle$ is discontinuous. Note that J is given by the partition function Z_L and $\langle\rho\rangle$ is given by the first derivative of Z_L. Then, in the terminology of statistical mechanics, we can say the transition is of first order across the line between phases A and B, and is of second order across the line between phases A and C, or phases B and C.

It is interesting to discuss some extreme limit cases. When $q > 1$ and $\delta = 0$, or equivalently $d = 0$, the situation is that there is no particle supply at the right boundary. Since the particles are likely to move leftward in the bulk and can move out the system at the left boundary, the system becomes short of particles in the end. In this extreme case, as remarked at the end of section 3 the weight function in the integral should be changed to the form of (3.24). The partition function Z_L is then

$$Z_L = \int_{-\infty}^{\infty} \frac{\mathrm{d}u}{\log q} \frac{(\mathrm{i}aq^{-1}\,\mathrm{e}^{u}, -\mathrm{i}aq^{-1}\,\mathrm{e}^{-u}, \mathrm{i}bq^{-1}\,\mathrm{e}^{u}, -\mathrm{i}bq^{-1}\,\mathrm{e}^{-u}, \mathrm{i}cq^{-1}\,\mathrm{e}^{u}, -\mathrm{i}cq^{-1}\,\mathrm{e}^{-u}; q^{-1})_\infty}{(-q^{-1}\,\mathrm{e}^{2u}, -q^{-1}\,\mathrm{e}^{-2u}; q^{-1})_\infty} \times \left[\frac{2+2\mathrm{i}\sinh u}{1-q}\right]^L. \tag{6.15}$$

Similarly, when $q > 1$ and $\gamma = 0$, or equivalently $c = 0$, the situation is that there is no escape of particles at the left boundary. More and more particles accumulate near the left 'blocking' boundary and finally the system is stopped with jammed particles. The partition function in this case is almost the same as above. Just replace c by d. We remark that the case where $q > 1$ and $c = d = 0$ (or, $\gamma = \delta = 0$) was treated in [17]

6.2. *The case where $q = 1$*

The partition function for $q = 1$ is given by

$$Z_L = \frac{1}{\Gamma(\lambda+1)} \int_0^\infty \mathrm{d}x\, x^{\lambda+L}\,\mathrm{e}^{-x} = \frac{\Gamma(\lambda+L+1)}{\Gamma(\lambda+1)}. \tag{6.16}$$

The current is calculated as

$$J = \frac{1}{\lambda+L}. \tag{6.17}$$

Instead of the average density (2.13), we compute exactly the particle density profile $\langle\tau_k\rangle$ in the next section.

7. The *n*-point function

The n-point functions are also obtained in integral form. In general, we find that the n-point function contains $n + 1$-multiple integrals.

7.1. *The case where $q \neq 1$*

Inserting the identity operator (4.27) $n + 1$ times altogether between D in the matrix products expression and using the form factor (4.32), we obtain the n-point function for $j_1 < \cdots < j_n$,

$$\begin{aligned}\langle\tau_{j_1}\cdots\tau_{j_n}\rangle = {}& \frac{1}{(1-q)^L Z_L} \lim_{\xi_1,\ldots,\xi_n\to 1} \left[\prod_{m=1}^{n+1} \oint_{C_m} \frac{\mathrm{d}z_m}{4\pi\mathrm{i}z_m}\right] \\ & \times \frac{\prod_{m=1}^{n+1} \left(z_m^2, z_m^{-2}; q\right)_\infty [(1+z_m)(1+1/z_m)]^{j_m-j_{m-1}-1}}{(az_1, a/z_1, cz_1, c/z_1, bz_{n+1}, b/z_{n+1}, dz_{n+1}, d/z_{n+1}; q)_\infty} \\ & \times \prod_{m=1}^{n} \left[\frac{1}{\left(z_m^2, z_m^{-2}; q\right)_\infty}\delta(z_{m+1}-z_m)\right. \\ & \left. + \frac{(q;q)_\infty^2 (z_{m+1}+1/z_{m+1}-\xi_m z_m - \xi_m/z_m)}{(\xi_m z_m z_{m+1}, \xi_m z_m/z_{m+1}, \xi_m z_{m+1}/z_m, \xi_m/z_m z_{m+1}; q)_\infty}\right].\end{aligned} \tag{7.1}$$

where $j_0 = 0$, $j_{n+1} = L + 1$ in the product. Regularization parameters ξ_m are included since otherwise this integral becomes a singular integral. The contour $C_m (m = 2, \ldots, n + 1)$ encloses the poles at $z_m = \xi_{m-1}z_{m-1}q^k, \xi_{m-1}z_{m-1}^{-1}q^k$ $(k \in \mathbb{Z}_+)$ and excludes the poles at $z_m = (\xi_{m-1}z_{m-1}q^k)^{-1}, \left(\xi_{m-1}z_{m-1}^{-1}q^k\right)^{-1}$ $(k \in \mathbb{Z}_+)$. In addition, for $m = 1$, C_1 encloses the poles at $z_1 = aq^k, cq^k$ $(k \in \mathbb{Z}_+)$ and excludes the poles at $z_1 = (aq^k)^{-1}, (cq^k)^{-1}$ $(k \in \mathbb{Z}_+)$. Also, C_{n+1} encloses the poles at $z_{n+1} = bq^k, dq^k$ $(k \in \mathbb{Z}_+)$ and excludes the poles at $z_{n+1} = (bq^k)^{-1}, (dq^k)^{-1}$ $(k \in \mathbb{Z}_+)$. Note that the result should be independent of the order of insertion of the identity operator. The above choice of integral contours corresponds to the case when the insertions are done from left to right.

The results for the $q > 1$ case are simply obtained from the reflection symmetry (4.4).

7.2. The case where $q = 1$

Applying formulae in section 5, we also obtain the n-point function for $q = 1$:

$$\langle \tau_{j_1} \cdots \tau_{j_n} \rangle = \frac{1}{\mu Z_L} \lim_{\xi_1,\dots,\xi_n \to 1} \left[\prod_{m=1}^{n+1} \int_0^\infty \mathrm{d}x_m \, x_m^{\lambda} \, \mathrm{e}^{-x_m} \right] \prod_{m=1}^{n+1} x_m^{j_m - j_{m-1} - 1}$$
$$\times \prod_{m=1}^{n} \left[(c_1 + c_2 x_m) x_m^{-\lambda} \, \mathrm{e}^{x_m} \delta(x_{m+1} - x_m) + c_3 \mathcal{J}(x_m, x_{m+1}, \xi_m) \right] \tag{7.2}$$

where $j_0 = 0$, $j_{n+1} = L+1$ in the product. In particular, for the one-point function the integral can be performed directly. Thus, we obtain

$$\langle \tau_k \rangle = \frac{\alpha}{\alpha + \gamma} - \frac{1}{\lambda + L} \frac{\alpha\beta - \gamma\delta}{(\alpha + \gamma)(\beta + \delta)} \left(\frac{1}{\alpha + \gamma} + k - 1 \right) \tag{7.3}$$

for $k = 1, \dots, L$. This shows a linear profile of particle density.

8. Conclusion

We have studied the steady state of the ASEP for the most general case of open boundary conditions where particles hop in both directions and are injected and ejected at both boundaries. Finding an explicit representation of the algebraic relations related to the Askey–Wilson polynomials, we have obtained the partition function in the form of the moments with respect to the weight function of the Askey–Wilson polynomials. This is an extension of the previous work for two degrees of freedom to the most general case. Furthermore, we also have found a novel integral formula for the n-point functions. We have emphasized that the finally obtained integral formulae are independent of our approach here and what we have also clarified is that the origin of the weight function is understood from the explicit representation of the matrices in the matrix method and its close relation to the Askey–Wilson polynomial.

The integral formulae themselves are important in analysing the properties of the steady state. For one thing, from the asymptotic behaviour of their partition function, the current in the thermodynamic limit has been calculated. The phase diagram is given and the boundary-induced phase transitions are observed. For the n-point functions, a limit procedure is included in the multiple integrals. Their asymptotic evaluation is more difficult, but could be done by generalizing the methods in [18].

The advantage of our method using the orthogonal polynomials is that, once the corresponding polynomials are known, one can use the whole storage of knowledge on them. It should be stressed that the Askey–Wilson polynomials are considered to be some of the most important orthogonal polynomials because all important classical orthogonal polynomials are obtained as special/limiting cases of the Askey–Wilson polynomials.

The discovery of the connection to the Askey–Wilson polynomials is yet more evidence of a deep mathematical structure of the ASEP, which has been already suggested in several previous works. The ASEP can be considered as an exactly solvable spin system and one may apply the standard techniques in the field, for instance, the Bethe ansatz. Whereas the matrix method is mainly suited for the study of stationary states, the Bethe ansatz is a powerful method in investigating the spectrum and the excited states of the model. In fact, it has allowed us to obtain some dynamical properties of the ASEP on a periodic or an infinite lattice [30, 31]. There have been several attempts to find the relationship between the Bethe ansatz method and the matrix method [32]. So far, however, it remains difficult to fully utilize the relationship and study the dynamical properties for the open boundary case. It is also noted that the connection of these methods through the Zamolodchikov–Faddeev algebra is pointed out in [33]. In addition, more recently, fluctuations of the current of the ASEP have been studied using the connection to the random matrix theory [34, 35]. It would be of great interest to further clarify the interrelationship among these fascinating connections.

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