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Exact solution of a partially asymmetric exclusion model using a deformed oscillator algebra

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Abstract. We study the partially asymmetric exclusion process with open boundaries. We generalize the matrix approach previously used to solve the special case of total asymmetry and derive exact expressions for the partition sum and currents valid for all values of the asymmetry parameter q. Due to the relationship between the matrix algebra and the q-deformed quantum harmonic oscillator algebra we find that q-Hermite polynomials, along with their orthogonality properties and generating functions, are of great utility. We employ two distinct sets of q-Hermite polynomials, one for $q < 1$ and the other for $q > 1$. It turns out that these correspond to two distinct regimes: the previously studied case of forward bias ($q < 1$) and the regime of reverse bias ($q > 1$) where the boundaries support a current opposite in direction to the bulk bias. For the forward bias case we confirm the previously proposed phase diagram whereas the case of reverse bias produces a new phase in which the current decreases exponentially with system size.

1. Introduction

The asymmetric simple exclusion process (ASEP) [1] is a much studied model from both mathematical and physical viewpoints. The model comprises particles hopping in a preferred direction on a lattice with hard-core exclusion imposed. In the mathematical literature the interest lies in it being a simple realization of interacting Markov processes [2] and much progress has been made in proving existence theorems, invariant measures and hydrodynamic limits [1]. Early applications concerned biophysical problems such as single-filing constraint in transport across membranes [3] and the kinetics of biopolymerization [4]. More recently the ASEP has achieved the status of a fundamental non-equilibrium model due to its intimate relation to growth phenomena and the KPZ equation [5], the problem of directed polymers in a random media [6] and its use as a microscopic model for driven diffusive systems [7] and shock formation [8]. Last but not least, many traffic flow models are based on variants of the ASEP [9]. Adding to its appeal is the fact that many exact results have been obtained, particularly in one dimension, allowing an analytical understanding of the non-equilibrium phenomena exhibited [10].

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In recent years the open boundary problem, where particles attempt to enter at the left of a one-dimensional lattice of N sites with rate α, hop to the right under a hard-core exclusion constraint and exit at the right with rate β, has been of considerable interest. It was first pointed out by Krug that boundary-induced phase transitions can occur [11] and it has further been shown that spontaneous symmetry breaking takes place when two oppositely moving particle species are introduced [12].

The door was opened to the analytical study of the open boundary model and its non-equilibrium steady state in [13]. There, exact recursion relations on the steady-state weights were obtained and density profiles and currents were worked out exactly for the case $\alpha = \beta = 1$. Also a mean field phase diagram in the α–β plane was derived. Then the recursion relations were used to calculate correlation functions for the case $\alpha = \beta = 1$ [14]. In [15] a different method, to be referred to as the matrix approach, was proposed: it was shown that the steady-state weights can written as a product of matrices which are in general of infinite dimension and non-commuting. The matrices obey algebraic rules which replace the recursion relations found in [13]. This approach gives the full solution of the model including the phase diagram and density profiles and allows, in principle, calculation of all equal time correlation functions. Further it admits generalization to other models. It should be noted that the phase diagram and density profiles were also obtained independently working from the recursion relations [16]. Subsequently the matrix approach has been used to solve new models with several species [17–20] and various updating schemes [21–23], to calculate shock profiles on an infinite system [24] and to recover some previously known results [25].

The phase diagram obtained for the one-species open boundary case [13,15,16] comprises three phases: a low-density phase, a high-density phase and a maximal current phase where generic long-range correlations occur. This phase diagram appears quite robust for driven diffusive systems with open boundaries [26]. Also it has been shown that different types of updates the same generic phase diagram pertains, except in simple cases of deterministic bulk dynamics where the maximal current phase is absent [27,28].

The partially asymmetric exclusion process is a generalization of the model where particles are able to hop to the left as well as to the right. The case of partial asymmetry is of interest since it allows one to interpolate between symmetric exclusion which can have equilibrium steady states and the far-from equilibrium asymmetric system. In the context of growth phenomena the two different systems are described by Edwards–Wilkinson and KPZ universality classes [11] and the crossover phenomena has been of interest [29,30].

A parameter q gives the ratio of hopping rates to the left and to the right; thus $q = 0$ recovers the totally asymmetric process and $q = 1$ gives the fully symmetric case. Furthermore, in the range $0 < q < 1$ there exists what we shall refer to as the *forward bias* regime where particles hop preferentially to the right and the boundary conditions are such that a steady-state current of particles to the right is supported. In contrast, when $q > 1$ particles can only enter at the left and leave at the right but hop preferentially to the left in the bulk. A steady-state current of particles to the right can then be supported by the boundary conditions *against* the bulk bias. This gives rise to a new phase which we analyse for the first time here. We show that the current decreases exponentially with the length of the system. This phase is of interest in the context of 'backbend dynamics' [31,32] where, for example, a fluid in a permeable medium has to traverse a pore oriented against the direction of gravity. It also appears that such a reverse bias phase is relevant to recently reported one-dimensional phase separation [19,33].

In [15] the generalization of the matrix approach to the partially asymmetric exclusion process was pointed out. This was used in [34] to obtain approximate expressions for the current in the forward bias case for large system size. It was also pointed out that the matrices for the partially asymmetric case are closely related to creation and annihilation operators of the q-deformed harmonic oscillator. In [35] the quadratic algebra was studied and curves in the parameter space were deduced for which finite matrices could be used. Along these curves exact expressions for physical quantities, such as the current and correlation length, can be computed easily. Also, in the symmetric case $q = 1$ the steady state is straightforward to solve [36–38]. However, exact expressions for all system sizes and parameters have remained elusive.

In this work we build on the relationship of the quadratic algebra with the q-deformed harmonic oscillator algebra to calculate exact expressions for the current for all system sizes and parameter values. The basic approach is to use known properties, such as orthogonality and generating functions, of the q-deformed Hermite polynomials associated with the quadratic algebra.

This method was employed independently by [39] to study the case of forward bias ($q < 1$) and a phase diagram for this regime was obtained by examining the asymptotics of the normalization (partition sum). We have been able to consider for the first time the case $q > 1$ for which a less well known set of q-Hermite polynomials is required [40]. Furthermore we obtain as a main new result of our work an exact, explicit expression for the normalization valid for *all* q which encompasses all regimes: $q = 0$ (total asymmetry), $q < 1$ (forward bias), $q = 1$ (symmetric) and $q > 1$ (reverse bias). This exact expression allows all physical quantities of the model to be evaluated for any system size and we use it here to obtain the asymptotic form of the current in the reverse bias regime.

The paper is organized as follows: in section 2 we define the model we consider and in section 3 we review the matrix approach and the related quadratic algebra. In section 4 we discuss the q-deformed harmonic oscillator and its relation to the quadratic algebra of the present problem. In particular, we present relevant facts such as the generating functions and orthogonality relations for the q-Hermite polynomials. In section 5 we derive our main results, which are exact expressions for the normalization (partition sum). In section 5.1 we derive an integral expression valid for $q < 1$ (41) and in section 5.2 we derive an integral expression valid for $q > 1$ (43). We then obtain in section 5.3 a finite sum expression valid for all q (57). In section 6 we use the exact expressions to calculate the asymptotic behaviour of the current and the phase diagram. We conclude in section 7 with a discussion.

2. Model definition

The microscopic dynamics of the model are specified by four rates at which certain events can occur. For a rate λ associated with a particular event, the probability that the event happens in an infinitesimal time interval dt is λdt. Furthermore, moves that would lead to two particles simultaneously occupying a single lattice site are prohibited due to the hard-core repulsion between them.

The events defined in the model and the rates at which they take place are as follows.

Event	*Rate*
Particle inserted onto the left boundary site	α
Particle removed from the right boundary site	β
Particle hops by one site to the right	1
Particle hops by one site to the left	q

Figure 1 shows a typical particle configuration on a small lattice along with the allowed moves and their rates.

As only three of the rates are independent, we have set the right hopping rate to 1 with no loss of generality in the following analysis.

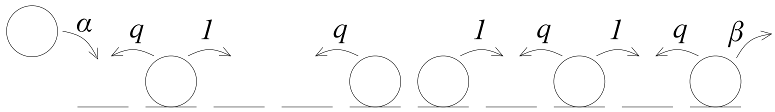

Figure 1. A typical particle configuration and allowed moves in the model.

Later, in section 7, we will consider a more general parameter space where particles can also enter at the right and exit at the left.

3. The matrix product formulation and its quadratic algebra

In this section we review the matrix approach to finding the steady state of the model. We present here the bare essentials of the method and refer the reader elsewhere for more detailed descriptions of the technique [10, 15, 41].

Consider first a configuration of particles $\mathcal{C}$ and its steady-state probability $P(\mathcal{C})$. We use as an ansatz for $P(\mathcal{C})$ an ordered product of matrices $X_1X_2\ldots X_N$ where $X_i = D$ if site i is occupied and $X_i = E$ if it is empty. To obtain a probability (a scalar value) from this matrix product, we employ two vectors $\langle W|$ and $|V\rangle$ in the following way:

$$P(\mathcal{C}) = \frac{\langle W|X_1X_2\ldots X_N|V\rangle}{Z_N}. \tag{1}$$

The factor Z_N is included to ensure that $P(\mathcal{C})$ is properly normalized. This latter quantity, analogous to a partition function, has the following simple matrix expression through which a new matrix C is defined:

$$Z_N = \langle W|(D+E)^N|V\rangle = \langle W|C^N|V\rangle. \tag{2}$$

Note that if D and E do not commute $P(\mathcal{C})$ is a function of both the number and position of particles on the lattice, as expected for a non-trivial steady state. The algebraic properties of the matrices can be deduced from the master equation for the process [15]. It can be shown that sufficient conditions for equation (1) to hold are

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

$$\alpha\langle W|E = \langle W| \tag{4}$$

$$\beta D|V\rangle = |V\rangle. \tag{5}$$

One can also write expressions for ensemble-averaged quantities in terms of matrix products. For example the current of particles J through the bond between sites i and $i+1$ is given by

$$J = \frac{\langle W|C^{i-1}(DE-qED)C^{N-i-1}|V\rangle}{Z_N} = \frac{Z_{N-1}}{Z_N} \tag{6}$$

where the last equality follows from relation (3). We see that, as expected in the steady state, the current is independent of the bond chosen. Also, the mean occupation number (density) of site i may be written as

$$\tau_i = \frac{\langle W|C^{i-1}DC^{N-i}|V\rangle}{Z_N}. \tag{7}$$

Our task now is to evaluate the matrix products in the above expressions for Z_N, J and τ_i by applying the rules (3)–(5).

In [15] the case $q = 0$ was treated by using (3) repeatedly to 'normal-order' matrix products: that is, to obtain an equivalent sum of products in which all E matrices appear to the left of any D matrices. Then finding a scalar value from (4) and (5) is straightforward. For example one can develop (2) as

$$Z_N = \langle W|C^N|V\rangle = \sum_{n,m} a_{N,n,m}\langle W|E^n D^m|V\rangle = \langle W|V\rangle \sum_{n,m} a_{N,n,m}\alpha^{-n}\beta^{-m}. \tag{8}$$

The difficulty with this approach lies in the combinatorial problem of finding the coefficients $a_{N,n,m}$. An alternative approach proposed in [15] is to find an explicit representation of C and decompose the vectors $\langle W|$ and $|V\rangle$ onto the eigenbasis of C to evaluate the normalization.

In the present work we employ mainly the latter approach to derive an expression for the normalization which is valid over a restricted range of the model parameters. We will later compare this with the canonical form (8) to find an expression which does not depend on the chosen representation and is therefore generally valid. The representation of C that we use is intimately related to the q-oscillator algebra and the eigenbasis of C is constructed from q-Hermite polynomials.

4. The q-deformed harmonic oscillator and its relevance

Much progress can be made if the algebra of the previous section is written in terms of that of q-deformed quantum harmonic oscillator [42]. The relationship central to this algebra is the q-deformed commutator

$$\hat{a}\hat{a}^\dagger - q\hat{a}^\dagger\hat{a} = \mathbb{1} \tag{9}$$

where the operators $\hat{a}$ and $\hat{a}^\dagger$ operate on basis vectors $|n\rangle$ (with $n = 0, 1, 2, \ldots$) as follows:

$$\hat{a}^\dagger|n\rangle = \left(\frac{1-q^{n+1}}{1-q}\right)^{\frac{1}{2}} |n+1\rangle \tag{10}$$

$$\hat{a}|n\rangle = \left(\frac{1-q^{n}}{1-q}\right)^{\frac{1}{2}} |n-1\rangle \tag{11}$$

$$\hat{a}|0\rangle = 0. \tag{12}$$

In terms of these new operators, the matrices introduced in the previous section can be written as

$$D = \frac{1}{1-q} + \frac{1}{\sqrt{1-q}}\hat{a} \tag{13}$$

$$E = \frac{1}{1-q} + \frac{1}{\sqrt{1-q}}\hat{a}^\dagger \tag{14}$$

and one finds using (9) that (3) is satisfied.

We now have an explicit representation of the original D and E matrices in the oscillator's 'energy' eigenbasis $\{|n\rangle\}$. Thus one may combine equations (13), (11) and (5) to find the corresponding representation of the vector $|V\rangle$:

$$\langle n|V\rangle = \frac{v^n}{\prod_{j=1}^{n}\sqrt{(1-q^j)}} \tag{15}$$

where we have set $\langle 0|V\rangle = 1$ and v is the following combination of the model parameters:

$$v = \frac{1-q}{\beta} - 1. \tag{16}$$

The denominator of (15) is more conveniently written in terms of a 'q-shifted factorial'. This is defined through

$$(a;q)_n = \prod_{j=0}^{n-1}(1-aq^j) \tag{17}$$

$$(a;q)_0 = 1. \tag{18}$$

We will later encounter products of these factorials for which we shall use the shorthand notation employed by [43]:

$$(a,b,c,\ldots;q)_n = (a;q)_n(b;q)_n(c;q)_n\ldots. \tag{19}$$

We can now use this compact notation to write expressions for both $\langle n|V\rangle$ and $\langle W|n\rangle$, the route to the latter being the same as that to find $\langle n|V\rangle$:

$$\langle n|V\rangle = \frac{v^n}{\sqrt{(q;q)_n}} \tag{20}$$

$$\langle W|n\rangle = \frac{w^n}{\sqrt{(q;q)_n}} \tag{21}$$

where v is given by (16) and

$$w = \frac{1-q}{\alpha} - 1. \tag{22}$$

We see that the representation of D and E (13) and (14) breaks down for certain choices of the model parameters. Firstly, for $q = 1$ (symmetric exclusion) a number of singularities appear. Secondly, if $v > 1$ and $q < 1$, the vector element $\langle n|V\rangle$ (20) is unbounded from above as $n \to \infty$; similarly with $\langle W|n\rangle$ (21) when $w > 1$ and $q < 1$. We consider for the moment only those regions of parameter space where this representation converges, and discuss the generalization to the remaining areas in section 5.3.

We persevere with the relationship between the original quadratic algebra and the q-oscillator algebra for the reason we now explain. We introduced earlier a matrix C which appears in the expressions for the mean particle density and current. We now see that this matrix can be written as a linear combination of the identity $\mathbb{1}$ and the 'coordinate' operator $\hat{x} = \hat{a} + \hat{a}^\dagger$:

$$C = D + E = \frac{2}{1-q}\mathbb{1} + \frac{1}{\sqrt{1-q}}\hat{x}. \tag{23}$$

The eigenstates of the oscillator in the coordinate representation are known—in analogy with the solutions of the undeformed oscillator they are called the continuous q-Hermite polynomials [43]. Clearly, the eigenvectors of C are the same as those for $\hat{x}$ and therefore knowledge of them permits diagonalization of C. As this is a major step towards obtaining the exact solution of the model, it is worth spending a little time discussing the q-Hermite polynomials.

The recursion relation for the polynomials follows after a suitable definition of the operator $\hat{x}$ on its eigenbasis $\{|x\rangle\}$:

$$\hat{x}|x\rangle = \frac{2x}{\sqrt{1-q}}|x\rangle. \tag{24}$$

From this and equations (11) and (10) we find

$$2x\langle x|n\rangle = \sqrt{1-q^n}\langle x|n-1\rangle + \sqrt{1-q^{n+1}}\langle x|n+1\rangle. \tag{25}$$

Explicit formulae for $\langle x|n\rangle$ can be found using a generating function technique, the details of which differ slightly depending on whether $q < 1$ or $q > 1$. Here we present the results which will be most useful later; derivations are given in appendix A.

When $q < 1$ we make a change of variable

$$x = \cos\theta. \tag{26}$$

The q-Hermite polynomials can now be defined as $\langle\theta|n\rangle$, that is, the projection of the oscillator energy eigenstate $|n\rangle$ onto the position basis $\langle\theta|$. The generating function

$$G(\theta,\lambda) = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{(q;q)_n}} \langle\theta|n\rangle \tag{27}$$

can be expressed as an infinite product

$$G(\theta,\lambda) = \frac{1}{(\lambda\mathrm{e}^{\mathrm{i}\theta}, \lambda\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty} \tag{28}$$

when $|\lambda| < 1$. An explicit form of the q-Hermite polynomial $\langle\theta|n\rangle$ can be determined from the generating function and is presented in appendix A, equation (A.6). It can also be shown [43] that the set of q-Hermite polynomials are orthogonal with respect to a weight function $\nu(\theta)$. That is

$$\int_0^\pi \mathrm{d}\theta \langle n|\theta\rangle \nu(\theta) \langle\theta|m\rangle = \delta_{n,m} \tag{29}$$

where

$$\nu(\theta) = \frac{(q, \mathrm{e}^{2\mathrm{i}\theta}, \mathrm{e}^{-2\mathrm{i}\theta}; q)_\infty}{2\pi}. \tag{30}$$

Similar results emerge when $q > 1$ under a different change of variable

$$x = \mathrm{i}\sinh u \tag{31}$$

with a suitably redefined generating function valid for all λ:

$$G(u,\lambda) = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{(q;q)_n}} \langle u|n\rangle = (\mathrm{i}q^{-1}\lambda\mathrm{e}^{u}, -\mathrm{i}q^{-1}\lambda\mathrm{e}^{-u}; q^{-1})_\infty. \tag{32}$$

An explicit expression for $\langle u|n\rangle$ is given in (A.10). Again a weight function $\nu(u)$ that orthogonalizes the polynomials can be found [40]. We write

$$\int_{-\infty}^{\infty} \mathrm{d}u \langle n|u\rangle \nu(u) \langle u|m\rangle = \delta_{n,m} \tag{33}$$

where now

$$\nu(u) = \frac{1}{\ln q} \frac{1}{(q^{-1}, -q^{-1}\mathrm{e}^{2u}, -q^{-1}\mathrm{e}^{-2u}; q^{-1})_\infty}. \tag{34}$$

5. Exact expressions for the normalization Z_N

5.1. Integral representation for $q < 1$

The relationships in the previous section allow us to obtain integral representations of matrix products. Here we illustrate how to apply the procedure to obtain an expression for the normalization Z_N when $q < 1$. The procedure used to obtain this particular result is also described by [39]; in the next section we extend the method to the case $q > 1$.

First we take the orthogonality relation for the q-Hermite polynomials (29) and use it to form a representation of the identity matrix:

$$\int_0^\pi \mathrm{d}\theta |\theta\rangle \nu(\theta) \langle\theta| = \mathbb{1}. \tag{35}$$

We now insert this into the expression for the normalization (2):

$$Z_N = \int_0^\pi \mathrm{d}\theta\, \nu(\theta) \langle W|C^N|\theta\rangle\langle\theta|V\rangle. \tag{36}$$

By design, the matrix C is acting on its eigenvectors, so using (23) and (26) we obtain

$$Z_N = \int_0^\pi \mathrm{d}\theta\, \nu(\theta) \langle W|\theta\rangle \left(\frac{2(\cos\theta + 1)}{1-q}\right)^N \langle\theta|V\rangle. \tag{37}$$

It is necessary to decompose the boundary vectors $\langle W|$ and $|V\rangle$ onto the $\{|\theta\rangle\}$ basis. By inserting a complete set of the basis vectors $\{|n\rangle\}$ we find

$$\langle\theta|V\rangle = \sum_{n=0}^\infty \langle\theta|n\rangle\langle n|V\rangle = \sum_{n=0}^\infty \frac{v^n}{\sqrt{(q;q)_n}} \langle\theta|n\rangle. \tag{38}$$

The final sum in this equation is just the generating function of the q-Hermite polynomials (27). Thus, when $|v| < 1$, we may write

$$\langle\theta|V\rangle = G(\theta, v) = \frac{1}{(v\mathrm{e}^{\mathrm{i}\theta}, v\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}. \tag{39}$$

Similarly, when $|w| < 1$ we find

$$\langle W|\theta\rangle = G(\theta, w) = \frac{1}{(w\mathrm{e}^{\mathrm{i}\theta}, w\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}. \tag{40}$$

Putting all this together, we arrive at an exact integral form for the normalization

$$Z_N = \left(\frac{1}{1-q}\right)^N \int_0^\pi \mathrm{d}\theta\, \nu(\theta)[2(1+\cos\theta)]^N G(\theta, w) G(\theta, v) \tag{41}$$

which, written out more fully, reads

$$Z_N = \frac{(q;q)_\infty}{2\pi} \left(\frac{1}{1-q}\right)^N \int_0^\pi \mathrm{d}\theta [2(1+\cos\theta)]^N \frac{(\mathrm{e}^{2\mathrm{i}\theta}, \mathrm{e}^{-2\mathrm{i}\theta}; q)_\infty}{(v\mathrm{e}^{\mathrm{i}\theta}, v\mathrm{e}^{-\mathrm{i}\theta}, w\mathrm{e}^{\mathrm{i}\theta}, w\mathrm{e}^{-\mathrm{i}\theta}; q)_\infty}. \tag{42}$$

When $|v| > 1$ or $|w| > 1$ equation (41) is not well-defined because $G(\theta, \lambda)$ does not converge when $|\lambda| > 1$. Rather than finding a representation of the quadratic algebra that does not suffer from this problem, one can simply analytically continue the integral (42) to obtain Z_N when $|v|$ or $|w|$ takes on a value greater than one. This procedure is carried out in section 6.

5.2. *Integral representation for $q > 1$*

We now apply the procedure of the previous section to find an integral representation of the normalization for the case of $q > 1$ which has not previously been considered. The only difference is that we must use the $q > 1$ forms of the generating function and weight function of the q-Hermite polynomials, namely equations (32)–(34). We obtain a similar form for Z_N to (41):

$$Z_N = \left(\frac{1}{1-q}\right)^N \int_{-\infty}^\infty \mathrm{d}u\, \nu(u)[2(1+\mathrm{i}\sinh u)]^N G(u, w) G(u, v). \tag{43}$$

However, the full form is somewhat different from (42):

$$Z_N = \frac{1}{\ln q}\frac{1}{(q^{-1};q^{-1})_\infty}\left(\frac{2}{1-q}\right)^N \int_{-\infty}^{\infty} \mathrm{d}u(1+\mathrm{i}\sinh u)^N \times \frac{(\mathrm{i}q^{-1}v\mathrm{e}^{u}, -\mathrm{i}q^{-1}v\mathrm{e}^{-u}, \mathrm{i}q^{-1}w\mathrm{e}^{u}, -\mathrm{i}q^{-1}w\mathrm{e}^{-u}; q^{-1})_\infty}{(-q^{-1}\mathrm{e}^{2u}, -q^{-1}\mathrm{e}^{-2u}; q^{-1})_\infty}. \tag{44}$$

One should note the range of integration is infinite and that, in contrast to equation (42), it cannot be simply replaced by a closed contour in the complex plane. It is this feature which makes this integral unsuited to approximation using the saddle-point method as we discuss in section 6.2.

5.3. Explicit formula

In this section we derive an alternative expression for Z_N which takes the form of a finite sum rather than an integral and is valid for all values of the model parameters. Such an expression is useful for two main reasons: firstly it allows us to extract the asymptotic form of the normalization when $q > 1$; secondly, as the sum contains a finite number of terms, it can be evaluated exactly by numerical means if one wishes to study finite-sized systems.

We will work from the integral for $q < 1$, $|v| < 1$ and $|w| < 1$ (41). The first stage of the calculation is to state an important identity:

$$\int_0^\pi \mathrm{d}\theta\, \nu(\theta)G(\theta,\lambda)G(\theta,v)G(\theta,w) = \frac{1}{(vw, \lambda v, \lambda w; q)_\infty}. \tag{45}$$

We do not prove this here but note that it is in fact a special case of the Askey–Wilson q-beta integral [43]†.

We now expand both sides of (45) in powers of λ. We already know the expansion of the left-hand side because $G(\theta,\lambda)$ is the generating function of the q-Hermite polynomials. The right-hand side may be treated by using another important identity valid when $|x| < 1$, $q < 1$ [43]:

$$\sum_{n=0}^{\infty}\frac{x^n}{(q;q)_n} = \frac{1}{(x;q)_\infty}. \tag{46}$$

We find

$$\frac{1}{(\lambda v, \lambda w; q)_\infty} = \sum_{n=0}^{\infty}\frac{\lambda^n}{(q;q)_n}\sum_{k=0}^{n}\begin{bmatrix} n \\ k \end{bmatrix}_q v^{n-k}w^k \tag{47}$$

where we have used the q-binomial coefficient which is

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \frac{(q;q)_n}{(q;q)_{n-k}(q;q)_k} \tag{48}$$

when $0 \leqslant k \leqslant n$ and zero otherwise. In the limit $q \to 1$ the q-binomial coefficient is equal to the conventional version $\binom{n}{k}$ familiar from combinatorics. Thus the last summation in (47) may be considered a q-deformation of the binomial expansion of $(v+w)^n$. We give this function the symbol $B_n(v,w;q)$:

$$B_n(v,w;q) = \sum_{k=0}^{n}\begin{bmatrix} n \\ k \end{bmatrix}_q v^{n-k}w^k. \tag{49}$$

† In its most general form the Askey–Wilson q-beta integral has four parameters, whereas identity (45) has only three.

If we now compare coefficients of powers of λ on both sides of (45) we obtain a key result:

$$\int_0^\pi \mathrm{d}\theta\, \nu(\theta)\langle\theta|n\rangle G(\theta, v)G(\theta, w) = \frac{1}{(vw;q)_\infty}\frac{B_n(v,w;q)}{\sqrt{(q;q)_n}}. \tag{50}$$

This relationship is important because we may take any sufficiently well-behaved function $f(\theta)$, re-express it it as a sum of q-Hermite polynomials and use (50) to evaluate the integral

$$\int_0^\pi \mathrm{d}\theta\, \nu(\theta) f(\theta) G(\theta, v)G(\theta, w). \tag{51}$$

Specifically, we can choose $f(\theta) = [2(1+\cos\theta)]^N$ and solve equation (41) exactly.

Expanding the cosine function in this way involves little more than routine algebra which is detailed in appendix B. The identity which emerges is

$$[2(1+\cos\theta)]^N = \sum_{n=0}^{N} R_{N,n}(q)\sqrt{(q;q)_n}\langle\theta|n\rangle \tag{52}$$

with

$$R_{N,n}(q) = \sum_{k=0}^{\lfloor\frac{N-n}{2}\rfloor} (-1)^k \binom{2N}{N-n-2k} q^{\binom{k}{2}} \left\{ \begin{bmatrix} n+k-1 \\ k-1 \end{bmatrix}_q + q^k \begin{bmatrix} n+k \\ k \end{bmatrix}_q \right\} \tag{53}$$

which may be alternatively written as

$$R_{N,n}(q) = \sum_{k=0}^{\lfloor\frac{N-n}{2}\rfloor} (-1)^k \left[\binom{2N}{N-n-2k} - \binom{2N}{N-n-2k-2} \right] q^{\binom{k+1}{2}} \begin{bmatrix} n+k \\ k \end{bmatrix}_q . \tag{54}$$

We may now insert the expansion (52) into (41) and integrate using (50):

$$Z_N = \frac{1}{(vw;q)_\infty}\left(\frac{1}{1-q}\right)^N \sum_{n=0}^{N} R_{N,n}(q) B_n(v,w;q). \tag{55}$$

This exact formula, valid for $q < 1$, $|v| < 1$ and $|w| < 1$ admits extension to general q, v and w. We first note that the infinite product in the prefactor can be replaced with $\langle W|V\rangle$, a fact which follows from (46):

$$\frac{1}{(vw;q)_\infty} = \sum_{n=0}^{\infty}\frac{(vw)^n}{(q;q)_n} = \langle W|V\rangle. \tag{56}$$

We claim that the resulting expression for the normalization

$$Z_N = \langle W|V\rangle \left(\frac{1}{1-q}\right)^N \sum_{n=0}^{N} R_{N,n}(q) B_n(v,w;q) \tag{57}$$

where $R_{N,n}(q)$ is given by (53) and $B_n(v,w;q)$ by (49), holds for *all* choices of the model parameters.

This is justified by observing that once v and w are written in terms of α and β using (16) and (22) we obtain a power series in α and β of the same form as (8). As discussed in section 3, an equation with this structure arises when one reorders a matrix product directly using the relation (3). To perform this direct manipulation, it is not necessary to employ a specific representation of the quadratic algebra. Therefore, although the representation we used to derive (57) breaks down for $q = 1$, $q < 1$, $|v| > 1$ or $q < 1$, $|w| > 1$, we can now say that had we used one which converges in the region of interest, we would still have obtained equation (57) for the normalization.

As a check of this formula, let us consider the case $q = 0$. Then (54) and (49) become

$$R_{N,n}(0) = \binom{2N}{N-n} - \binom{2N}{N-n-2} \tag{58}$$

$$B_n(v, w; 0) = \frac{v^{n+1} - w^{n+1}}{v - w} \tag{59}$$

where now $v = 1/\beta - 1$ and $w = 1/\alpha - 1$. It can be verified, using the identity

$$\sum_{n=r}^{X-Y} (-1)^n \binom{X}{Y-n} \binom{n}{r} = (-1)^r \binom{X-1-r}{Y-r} \tag{60}$$

that (57) can be rewritten as

$$Z_N = \langle W|V\rangle \sum_{k=0}^{N} \left[\binom{2N-2-k}{N-k} - \binom{2N-2-k}{N-2-k} \right] \left[\frac{(1/\beta)^{k+1} - (1/\alpha)^{k+1}}{1/\beta - 1/\alpha} \right] \tag{61}$$

which is equivalent to equation (39) of [15].

We note that for $q \to 1$ the singularity in the denominator of (57) is cancelled by the sum over $R_{N,n}(q) B_n(v, w; q)$ and the expression is in fact well behaved. Although we have checked for small system sizes that (57) agrees with the expression of [37] we have not been able to show this in a simple way.

6. The phase diagram of the model

We now have enough information to obtain an exact phase diagram for the model and expressions for the particle current in the large system size limit. The behaviour differs greatly according to whether the particles are forward biased ($q < 1$) or reverse biased ($q > 1$) and so we treat the two cases separately.

6.1. The forward bias regime

When $q < 1$, the quantities of interest are most quickly obtained from the integral (42) as was also done in [39]. As N becomes large, we can use the saddle-point method to evaluate Z_{N}, and so we rewrite (42) as a contour integral

$$Z_N = \frac{(q; q)_\infty}{4\pi \mathrm{i}} \left(\frac{1}{1-q} \right)^N \oint_K \frac{\mathrm{d}z}{z} (2 + z + z^{-1})^N \frac{(z^2, z^{-2}; q)_\infty}{(vz, wz, vz^{-1}, wz^{-1}; q)_\infty} \tag{62}$$

where the contour K is the circle $|z| = 1$ and is directed anti-clockwise. Furthermore it passes through the saddle-point of $2 + z + 1/z$ along the path of steepest descent. We find from the saddle-point formula that

$$Z_N \sim \frac{4}{\sqrt{\pi}} \frac{(q; q)_\infty^3}{(v, w; q)_\infty^2} \left(\frac{1}{N} \right)^{\frac{3}{2}} \left(\frac{4}{1-q} \right)^N \tag{63}$$

which holds as long as $|v| < 1$ and $|w| < 1$.

We can treat other values of v and w using the integral (62) after realizing that (63) gives the contribution from the contour K for any value of v and w, whereas the analytic continuation of Z_{N} is obtained by distorting the contour such that the poles at $z = v, qv, q^2v, \ldots$ and $z = w, qw, q^2w, \ldots$ stay inside it and all other poles are outside it. Figure 2 illustrates how to modify the contour as v is increased to a value $1 < v < 1/q$.

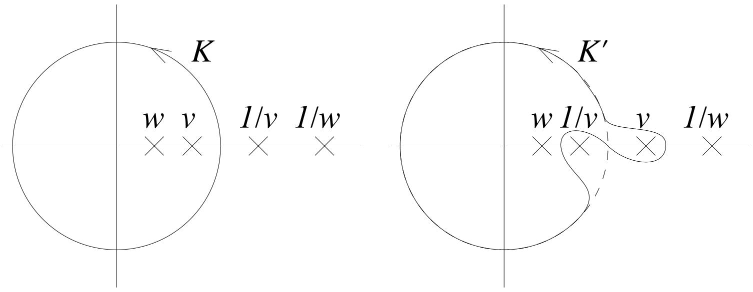

Figure 2. The integral over the contour K (shown dotted in the right-hand figure) can be determined from a saddle-point expansion, whereas the distorted contour K' is the correct one to use when $1 < v < 1/q$. Note that only the four poles closest to $z = 1$ have been shown for clarity.

Table 1. The normalization for different values of v and w when $q < 1$.

Region	Normalization Z_N
$v < 1, w < 1$	$\frac{4}{\sqrt{\pi}} \frac{(q;q)_\infty^3}{(v,w;q)_\infty^2} \left(\frac{1}{N}\right)^{\frac{3}{2}} \left(\frac{4}{1-q}\right)^N$
$v > w, v > 1$	$\frac{(v^{-2};q)_\infty}{(vw, w/v;q)_\infty} \left(\frac{2+v+v^{-1}}{1-q}\right)^N$
$w > v, w > 1$	$\frac{(w^{-2};q)_\infty}{(wv, v/w;q)_\infty} \left(\frac{2+w+w^{-1}}{1-q}\right)^N$

The difference between the two results can be calculated using the residue theorem. When $|w| < 1$, $1 < v < 1/q$ we find by looking at the poles at $z = v$ and $z = 1/v$ that we should add

$$\frac{(v^{-2};q)_\infty}{(vw, w/v;q)_\infty} \left(\frac{2+v+v^{-1}}{1-q}\right)^N \tag{64}$$

to (63). In the large-N limit, this correction dominates the contribution from the contour K and so we write

$$Z_N \sim \frac{(v^{-2};q)_\infty}{(vw, w/v;q)_\infty} \left(\frac{2+v+v^{-1}}{1-q}\right)^N \tag{65}$$

when $|w| < 1$ and $1 < v < 1/q$. As v is increased above $1/q$ and other poles need to be considered, (64) remains the dominant contribution to Z_N. One could guess this from the fact that the pole at $z = v$ is furthest from the origin.

Due to the symmetry of (62) in v and w, we obtain (65) with $v \leftrightarrow w$ when $w > 1$, $|v| < 1$. When both w and v are greater than one, the leading term in the asymptotic expansion comes, as before, from the pole furthest along the real axis of the complex plane. Thus we have found three different forms for Z_N, each of which corresponds to a phase in the model. These forms and their regions of validity are presented in table 1.

We can go on to find the currents in the three forward bias phases through equation (6). These expressions are presented in table 2. For completeness we should determine Z_N along each of the phase boundaries ($v = w > 1$ or $v = 1, w \neq 1$ etc). We find that the currents subsequently found are equal to the limiting values of those in table 2 as the boundary under consideration is approached from each of the neighbouring regions.

We can now draw a phase diagram for the system when $q < 1$: see figure 3. We note that it has the same structure as that found for $q = 0$ [15]. The region $|v| < 1$, $|w| < 1$ is

Table 2. The $N \to \infty$ forms of the particle current in the forward biased phases.

Region	Current J
$\alpha > \frac{1-q}{2}, \beta > \frac{1-q}{2}$	$\frac{1-q}{4}$
$\alpha < \frac{1-q}{2}, \beta > \alpha$	$\frac{\alpha(1-q-\alpha)}{1-q}$
$\beta < \frac{1-q}{2}, \alpha > \beta$	$\frac{\beta(1-q-\beta)}{1-q}$

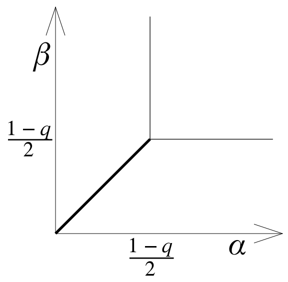

Figure 3. The phase diagram of the model when $q < 1$. The thick solid line is a first-order transition and the thin solid lines are second-order transitions in the sense of [15, 16].

a maximal current phase; the remaining two phases correspond to the high- and low-density phases found by [15]. Each of these two latter phases may be subdivided into three regions according to the behaviour of the density correlation length in the thermodynamic limit [39].

6.2. The reverse bias regime

We turn now to the case $q > 1$. We will show shortly by examining the exact formula (57) that the normalization behaves like $Z_{\mathrm{N}} \sim q^{\frac{1}{4}N^2}$ for large N. This sheds further light on why the saddle-point method is not applicable here: by its nature, it gives expressions where the exponent is linear in N rather than the desired quadratic.

To proceed we must find approximate forms of two elementary quantities: the q-shifted factorial and the q-binomial coefficient. We rewrite the definition (17) as

$$(q;q)_n = (-1)^n q^{\binom{n+1}{2}} \mathrm{e}^{M_n(q)} \tag{66}$$

where

$$M_n(q) = -\sum_{k=1}^{\infty} \frac{1}{k} \frac{1}{q^k - 1}(1 - q^{-kn}). \tag{67}$$

We see that when n is large, $M_n(q)$ can be approximated by

$$M(q) \simeq -\sum_{k=1}^{\infty} \frac{1}{k} \frac{1}{q^k - 1} \tag{68}$$

which is independent of n. This leads to an approximation of the q-binomial coefficient

$$\begin{bmatrix} n \\ k \end{bmatrix}_q \simeq q^{k(n-k)} \mathrm{e}^{-M(q)} \tag{69}$$

which is valid when both n and k are large. The rest of the analysis is not particularly illuminating, so is presented in appendix C. We ultimately find that when $q > 1$

$$Z_N \sim A(v, w; q)(q^{-1}vw, 1/vw; q^{-1})_\infty \left(\frac{\sqrt{vw}}{q-1}\right)^N q^{\frac{1}{4}N^2} \tag{70}$$

where

$$A(v, w; q) = \sqrt{\frac{\pi}{\ln q}} \exp\left\{M(q) + \frac{(\ln w/v)^2}{4\ln q}\right\}. \tag{71}$$

We should note that the smallest system size N for which (70) holds will be a function of q due to difference between the exact quantity $M_n(q)$ and the approximate form we used $M(q)$.

The expression for the current follows quickly from (6). This reads

$$J \sim \left(\frac{\alpha\beta(q-1)^2}{(q-1+\alpha)(q-1+\beta)}\right)^{\frac{1}{2}} q^{-\frac{1}{2}N+\frac{1}{4}} \tag{72}$$

which, in contrast with the currents in the forward bias regime, is a function of the number of lattice sites N.

7. Discussion

In this work we have employed properties of q-Hermite polynomials to calculate exact steady-state properties of the partially asymmetric exclusion process. The connection between this model and q-Hermite polynomials lies in the fact that the matrices D and E of the matrix product solution can be written in terms of q-raising and q-lowering operators as in (13). Then the calculation of the normalization (2) amounts to decomposing the vectors $\langle W|$ and $|V\rangle$ onto the eigenvectors of the matrix C which are the eigenvectors of the 'coordinate' operator of the q-deformed oscillator. This allowed us to obtain integral representations of the normalization for both the forward bias case $q < 1$ (41) and the reverse bias case $q > 1$ (43). Further we could use orthogonality properties of the q-Hermite polynomials to express these two integral expressions as a finite sum valid for all q (57).

In a very recent paper [39], orthogonal polynomials were also used to study the ASEP. In view of the fact that our work and [39] were carried out independently, a comparison is in order. In [39], the large system size limits of the normalization and the current in the forward bias regime $q < 1$ via the integral representation (41) were obtained. Furthermore it was shown that one could also analyse the density correlations from this integral. In this work we have found that a corresponding integral can also be found for the case of reverse bias $q > 1$. Further for all values of q (and α, β) we have succeeded in obtaining an exact sum formula valid for all system sizes. One application of this general expression was to calculate the current in the reverse bias phase.

For the forward bias case the phase diagram proposed by Sandow [34] is recovered. In that work the more general parameter space including rates γ (exit of particles at the left boundary) and δ (entry at the right) was considered. For this case the algebra is modified [15] to

$$DE - qED = D + E \tag{73}$$

$$\langle W|(\alpha E - \gamma D) = \langle W| \tag{74}$$

$$(\beta D - \delta E)|V\rangle = |V\rangle. \tag{75}$$

In principle we can generalize our method to that case, the only difference being that $\langle W|$ and $|V\rangle$ specified by (4) and (5) will have more complicated expressions than (20) and (21). In the forward bias case the generalization would not produce any new phases. However, for $q > 1$ allowing particles to exit at the left and enter at the right (both $\gamma, \delta > 0$) would allow a left flowing current of particles to be sustained, thus destroying the reverse bias phase.

The reverse bias phase where the boundary conditions impose a current opposite to the bulk bias realizes a new phase in the ASEP where the current decreases exponentially with system size. A typical arrangement of particles in this phase is a lattice full at the left end and empty at the right end. The form for the current $j \sim q^{-N/2}$ (72) suggests that the lattice is typically half full, i.e. the furthest particle to the right has typically to traverse a distance of $N/2$ sites against the bias to exit the lattice. To understand why the lattice is half full one invokes the particle hole symmetry that the current of particles exiting to the right must equal the current of holes exiting to the left. The symmetry implies that the lattice must be half full [31].

Further, for large N the current tends to zero and one can compare with the much simpler case where the current is exactly zero, for example when the boundaries are reflecting [44]. Then the microscopic dynamics obey detailed balance and the unnormalized probability of a configuration of M particles at positions $x_1, x_2, \ldots, x_M$ will be proportional to $q^{-\sum_{i=1}^{M} x_i}$. Here also the normalization grows exponentially in N^2 [33].

In a recent preprint [45] the density profiles for the three forward bias $q < 1$ phases were calculated in the thermodynamic limit. In particular in the maximal current phase it was shown that the density profile decays with distance x from the left boundary as $\frac{1}{2} + (4\pi x)^{-1/2}$ for large x. There remain, however, a number of issues to be resolved. As q tends to 1 the maximal current phase occupies more and more of the phase diagram—see figure 3. However, at $q = 1$ we know that the profile is exactly linear. This implies a non-trivial limit $q \to 1$ and therefore non-trivial crossover phenomena from the asymmetric to the symmetric case. This corresponds to the transition between KPZ and EW universality classes in the related growth models. Further in the reverse bias case ($q > 1$), as we expect the lattice to be roughly half full, the density profile should be sigmoid-like. For $q \to \infty$ the profile will be a sharp step function whereas as $q \to 1$ the sigmoid profile will straighten out into a linear profile.

It is known that the quadratic algebra (3)–(5) for the open boundary problem can be used to solve a partially asymmetric periodic system with the addition of defect particles [10, 17]. A defect particle hops forward with rate α but is overtaken (and moved back a site) by normal particles with rate β. When $q < 1$, the different phases in the present problem manifest themselves in this model [46]. However the case $q > 1$ is yet to be tackled; we believe this to be of special interest as the reverse bias phase corresponds to phase separation into pure domains and spontaneous breaking of translational invariance [19, 33].

Acknowledgments

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Appendix A. Generating functions of the q-Hermite polynomials

In this appendix we explain how to obtain the generating functions $G(\theta, \lambda)$ and $G(u, \lambda)$ from the recursion relations for the q-Hermite polynomials (25). We also present explicit expressions for the polynomials as they may be obtained easily from the generating functions.

We consider first a general form of G, suitable for both $q < 1$ and $q > 1$:

$$G(x, \lambda) = \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{(q; q)_n}} \langle x|n\rangle. \tag{A.1}$$

We now obtain a functional relation for $G(x, \lambda)$ by multiplying both sides of equation (25) by $\lambda^n/(\sqrt{(q; q)_n})$ and performing the required summations:

$$G(x, q\lambda) = (\lambda^2 - 2\lambda x + 1)G(x, \lambda). \tag{A.2}$$

By using this relation repeatedly, we can find an expression for $G(x,\lambda)$ in terms of $G(x,0)$. This latter quantity is fixed by normalization, and so we set it to 1.

It can be seen from (A.2) that our approach from $G(x,\lambda)$ to $G(x,0)$ depends on whether $q<1$ or $q>1$. Consider first the case $q<1$. It is useful to make the change of variable $x=\cos\theta$ so that (A.2) becomes

$$G(\theta,\lambda)=\frac{G(\theta,q\lambda)}{(1-\lambda\mathrm{e}^{\mathrm{i}\theta})(1-\lambda\mathrm{e}^{-\mathrm{i}\theta})}. \tag{A.3}$$

Iterating this we find

$$G(\theta,\lambda)=\frac{1}{(\lambda\mathrm{e}^{\mathrm{i}\theta},\lambda\mathrm{e}^{-\mathrm{i}\theta};q)_\infty} \tag{A.4}$$

where we have used $G(\theta,0)=1$. The infinite product $1/(x;q)_\infty$ has a well known series representation [43] valid for $x<1, q<1$

$$\frac{1}{(x;q)_\infty}=\sum_{n=0}^{\infty}\frac{x^n}{(q;q)_n} \tag{A.5}$$

from which we may extract the form of $\langle\theta|n\rangle$. Expanding both sides of (A.4) in λ and comparing coefficients we find

$$\langle\theta|n\rangle=\frac{1}{\sqrt{(q;q)_n}}\sum_{k=0}^{n}\begin{bmatrix} n\\ k\end{bmatrix}_q \mathrm{e}^{\mathrm{i}(n-2k)\theta} \tag{A.6}$$

where $\begin{bmatrix} n\\ k\end{bmatrix}_q$ is the q-deformed binomial described in section 5.3.

The case $q>1$ proceeds in the same way. We must however make a different change of variable $x=\mathrm{i}\sinh u$ because otherwise (24) would imply that we had found imaginary eigenvalues of a Hermitian matrix. Also we should divide λ by q in as we approach $G(u,0)$ from $G(u,\lambda)$. We thus rewrite (A.2) as

$$G(u,\lambda)=(1-\mathrm{i}q^{-1}\lambda\mathrm{e}^{u})(1+\mathrm{i}q^{-1}\lambda\mathrm{e}^{-u})G(u,q^{-1}\lambda) \tag{A.7}$$

and iterate before to obtain

$$G(u,\lambda)=(\mathrm{i}q^{-1}\lambda\mathrm{e}^{u},-\mathrm{i}q^{-1}\lambda\mathrm{e}^{-u};q^{-1})_\infty. \tag{A.8}$$

Again the infinite product on the right-hand side of this equation has a useful series expansion appropriate for $q>1$ and all x:

$$(q^{-1}x;q^{-1})_\infty=\sum_{n=0}^{\infty}\frac{x^n}{(q;q)_n}. \tag{A.9}$$

Expansion of (A.8) in powers of λ and comparison with the generating function (32) yields $\langle u|n\rangle$:

$$\langle u|n\rangle=\frac{\mathrm{i}^n}{\sqrt{(q;q)_n}}\sum_{k=0}^{n}(-1)^k\begin{bmatrix} n\\ k\end{bmatrix}_q \mathrm{e}^{(n-2k)u}. \tag{A.10}$$

It is important to realize that the two forms (A.6) and (A.10) we have found are not very different. In particular one can obtain the form (A.10) by making the substitution $\theta\to\pi/2-\mathrm{i}u$ which is another way of describing the replacement $\cos\theta\to\mathrm{i}\sinh u$. Also we should note that all the functions we have found are real on their domains despite the presence of i when $q>1$.

Appendix B. Expansion of the cosine function in q-Hermite polynomials

Here we show how to rewrite $[2(1+\cos\theta)]^N$ as a sum of q-Hermite polynomials $\langle\theta|n\rangle$. First of all we simplify the task by using an identity easily verified by induction:

$$[2(1+\cos\theta)]^N = \sum_{n=0}^{N} \binom{2N}{N-n} c_n(\theta) \tag{B.1}$$

with

$$c_n(\theta) = \begin{cases} 1 & n = 0 \\ 2\cos(n\theta) & n > 0. \end{cases} \tag{B.2}$$

We now need only to consider the expansion of $c_n(\theta)$. It is fairly easy to convince oneself by inspecting (A.6) that only those q-Hermite polynomials of the same parity as the cosine function c_n will appear in the expansion. Also we do not expect any contributions from $\langle\theta|k\rangle$ with $k > n$. This leads to the following prescription:

$$c_n(\theta) = \sum_{k=0}^{\lfloor\frac{n}{2}\rfloor} a_{n,k}\langle\theta|n-2k\rangle. \tag{B.3}$$

A formula for $a_{n,k}$ may be found by applying the orthogonality property of the q-Hermite polynomials (29). We obtain a familiar integral transform

$$a_{n,k} = \int_0^{\pi} \mathrm{d}\theta\ \nu(\theta)c_n(\theta)\langle n-2k|\theta\rangle. \tag{B.4}$$

To evaluate this integral we need the series expansion of the weight function $\nu(\theta)$

$$\nu(\theta) = \frac{1}{2\pi}\sum_{s=-\infty}^{\infty}(-)^s q^{\binom{s}{2}}\left(1+q^s\right)\mathrm{e}^{2\mathrm{i}s\theta} = \frac{1}{2\pi}\sum_{s=-\infty}^{\infty} b_s \mathrm{e}^{2\mathrm{i}s\theta}. \tag{B.5}$$

Inserting this and the explicit formula for the q-Hermite polynomial (A.6) into the above we find, after some manipulation,

$$a_{n,k} = \frac{1}{\sqrt{(q;q)_{n-2k}}}\sum_{s=-\infty}^{\infty} b_s \sum_{r=0}^{n-2k}\begin{bmatrix} n-2k \\ r \end{bmatrix}_q \frac{1}{2\pi}\int_0^{2\pi}\mathrm{d}\theta\ \cos((k+r-s)\theta). \tag{B.6}$$

The integral that appears in this equation is just a representation of the Kronecker delta symbol $\delta_{s,k+r}$. Thus we can eliminate the summation over s:

$$\begin{aligned} a_{n,k} &= \frac{(-1)^k}{\sqrt{(q;q)_{n-2k}}}\sum_{r=0}^{n-2k}\begin{bmatrix} n-2k \\ r \end{bmatrix}_q (-1)^r q^{\binom{k+r}{2}}(1+q^{k+r}) \\ &= \frac{(-1)^k q^{\binom{k}{2}}}{\sqrt{(q;q)_{n-2k}}}\sum_{r=0}^{n-2k}\begin{bmatrix} n-2k \\ r \end{bmatrix}_q (-1)^r q^{\binom{r}{2}+kr}(1+q^{k+r}) \\ &= \frac{(-1)^k q^{\binom{k}{2}}}{\sqrt{(q;q)_{n-2k}}}((q^k;q)_{n-2k} + q^k(q^{k+1};q)_{n-2k}). \end{aligned} \tag{B.7}$$

To do the last step, we have made used the following series expansion in x:

$$(x;q)_n = \sum_{k=0}^{n}\begin{bmatrix} n \\ k \end{bmatrix}_q (-1)^k q^{\binom{k}{2}} x^k. \tag{B.8}$$

The latest expression allows a little simplification by noting that

$$(aq^k;q)_{n-2k} = \frac{(a;q)_{n-k}}{(a;q)_k} \tag{B.9}$$

and so we find we find

$$a_{n,k} = (-1)^k \sqrt{(q;q)_{n-2k}} q^{\binom{k}{2}} \left(\begin{bmatrix} n-k-1 \\ k-1 \end{bmatrix}_q + q^k \begin{bmatrix} n-k \\ k \end{bmatrix}_q \right) \tag{B.10}$$

which is true for all n, k if we observe the usual convention that $\left[{n \atop k}\right]_q = 0$ when $k < 0$ or $k > n$.

We may now combine equations (B.1), (B.3) and (B.10) to find

$$\begin{aligned} [2(1+\cos\theta)]^N &= \sum_{n=0}^{N} \binom{2N}{N-n} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} a_{n,k} \langle \theta | n-2k \rangle \\ &= \sum_{n=0}^{N} \sum_{k=0}^{\lfloor \frac{N-n}{2} \rfloor} \binom{2N}{N-(n+2k)} a_{n+2k,k} \langle \theta | n \rangle \\ &= \sum_{n=0}^{N} R_{N,n}(q) \sqrt{(q;q)_n} \langle \theta | n \rangle \end{aligned} \tag{B.11}$$

thus completing the derivation of equation (52). The problem of expanding of a general function in q-Hermite polynomials was first solved by Rogers in 1894. His approach, detailed by [47], is more complicated than ours as he did not use the orthogonality properties of the q-Hermite polynomials.

Appendix C. Approximation of the normalization for large N and $q > 1$

We indicate here how to estimate Z_{N} as given by (57) in a systematic manner when N is large and $q > 1$. We begin with the function $B_n(v, w; q)$ which is defined by the sum in equation (49). The dominant terms are those around $k = n/2$, and so we may replace the q-binomial with the approximation (69) and also rewrite the sum as an integral over k. This gives for large n

$$B_n(v, w; q) \sim (-1)^n A(v, w; q) q^{\frac{1}{4}n^2} |vw|^{\frac{1}{2}n} \tag{C.1}$$

where $A(v, w; q)$ is given by (71).

We now consider the sum (53) for $R_{N,n}$. In this summation we keep only the term with largest k as the others are exponentially suppressed. We find then that

$$Z_N \simeq \frac{(q^{-1}vw; q^{-1})_\infty}{(1-q)^N} (S_N(v, w; q) + 2N S_{N-1}(v, w; q)) \tag{C.2}$$

where we have expanded the product $\langle W | V \rangle$ using the identity

$$\sum_{r=0}^{\infty} \frac{(qx)^r}{(q;q)_r} = (x; q^{-1})_\infty \tag{C.3}$$

which holds when $q > 1$ and for all x and where we have defined

$$S_N(v, w; q) = (1-q^N) \sum_{r=0}^{\lfloor \frac{N}{2} \rfloor} (-1)^r q^{\binom{r}{2}} \frac{(q;q)_{N-r-1}}{(q;q)_r (q;q)_{N-2r}} B_{N-2r}(v, w; q). \tag{C.4}$$

The main contribution to this latest sum $S_N(v, w; q)$ is where r is small. The approximation

$$(-1)^r q^{\binom{r}{2}} \frac{(q;q)_{N-r-1}}{(q;q)_r (q;q)_{N-2r}} \simeq -\frac{q^{-r^2+(N+1)r-N}}{(q;q)_r} \tag{C.5}$$

which follows from (66) and (68) is valid in that region and when combined with the asymptotic expression for $B_n(v, w; q)$ yields

$$S_N(v, w; q) \sim (-1)^N A(v, w; q)(1 - q^{-N})|vw|^{\frac{1}{2}N} q^{\frac{1}{4}N^2} \sum_{r=0}^{\lfloor \frac{N}{2} \rfloor} \frac{1}{(q; q)_r} \left(\frac{q}{vw}\right)^r . \tag{C.6}$$

We are now left with a single summation which may be estimated from the identity (C.3). We see

$$\sum_{r=0}^{\lfloor \frac{N}{2} \rfloor} \frac{1}{(q; q)_r} \left(\frac{q}{vw}\right)^r = (1/vw; q^{-1})_\infty + \mathcal{O}(q^{-\frac{1}{4}N^2}) \tag{C.7}$$

and so to leading order in q we find

$$S_N(v, w; q) \sim (-1)^N A(v, w; q)(1/vw; q^{-1})_\infty |vw|^{\frac{1}{2}N} q^{\frac{1}{4}N^2}. \tag{C.8}$$

Noting that S_{N-1} is exponentially smaller than S_N we may finally write down the asymptotic form of Z_{N} when $q > 1$

$$Z_N \sim A(v, w; q)(q^{-1}vw, 1/vw; q^{-1})_\infty \left(\frac{\sqrt{vw}}{q-1}\right)^N q^{\frac{1}{4}N^2} \tag{C.9}$$

which is the expression presented in section 6.2.

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