Bi-orthogonal polynomial sequences and the asymmetric simple exclusion process

R Brak and W Moore

Department of Mathematics, The University of Melbourne Parkville, Victoria 3052, Australia

E-mail: r.brak@ms.unimelb.edu.au

Received 28 September 2014, revised 22 June 2015
Accepted for publication 25 June 2015
Published 20 July 2015

Abstract
We state the diffusion algebra equations of the stationary state of the three parameter (α, β and q) asymmetric simple exclusion Process as a linear functional, \( \mathcal{L} \), acting on a tensor algebra. From \( \mathcal{L} \) we construct a pair of sequences, \( \{ P_n \} \) and \( \{ Q_m \} \), of monic polynomials which are bi-orthogonal, that is, they satisfy \( \mathcal{L}(P_n, Q_m) = \Lambda_n \delta_{n,m} \) (where \( \Lambda_n \) is a scalar). The uniqueness and existence of the pair of sequences arises from the determinant of the bi-moment matrix whose elements satisfy a pair of \( q \)-recurrence relations. The determinant is evaluated using an LDU-decomposition. If the linear functional is represented as an inner product, \( \mathcal{L}(\cdot, \cdot) = \langle W | V \rangle \) then the action of the polynomials \( Q_n \) on the boundary vector \( |V\rangle \) generate a basis \( \{ V_n \} = Q_n |V\rangle \) whose orthogonal dual vectors are given by the action of \( P_n \) on the dual boundary vector \( \langle W | \), that is \( \langle W_n | = \langle W | P_n \). This basis gives the representation of the algebra which is associated with the Al-Salam–Chihara polynomials obtained by Sasamoto.

Keywords: bi-orthogonal polynomials, orthogonal polynomials, asymmetric simple exclusion process, LDU-decomposition, diffusion algebra

(Some figures may appear in colour only in the online journal)

1. Introduction

The asymmetric simple exclusion process (ASEP) is a continuous time Markov process defined by particles hopping along a line of \( L \) sites—see figure 1. Particles hop on to the line on the left with rate \( \alpha \), off at the right with rate \( \beta \) and they hop to neighbouring sites to the left with rate \( q \) and rate one to the right with the constraint that only one particle can occupy a site.
The problem of computing the stationary probability distribution was solved by Derrida et al \cite{1} with the introduction of the matrix product Ansatz (see below) which provides an algebraic method of computing the stationary distribution. A recent review of the asymmetric exclusion process may be found in Blythe and Evans \cite{2}.

The matrix product Ansatz expresses the stationary distribution of a given state as an inner product on a certain quotient ring of matrices. This ring is generated by two matrices $D$ and $E$ which satisfy the relation

$$DE - qED - D - E = 0.$$ 

The inner product $\langle W | \cdot | V \rangle$ is then defined by two vectors $\langle W \rangle$ and $| V \rangle$ (which we will refer to as boundary vectors) which satisfy $(\beta D - 1)| V \rangle = 0$ and $(\alpha E - 1)\langle W \rangle = 0$.

Rather than using $D$ and $E$ the algebra is simplified by working with the shifted variables $d = q'D - 1, \quad e = q'E - 1,$

\begin{align}
\text{where } q' &= 1 - q. \text{ In these variables the above relation takes on the well known form (see for example, } [3] \text{)}
\end{align}

$$de - q ed = q'.$$

Computing representations of the $d$ and $e$ matrices falls into natural cases. The case with $\alpha$ and $\beta$ non-zero but $q = 0$ we will refer to as the two parameter model and the case $\alpha, \beta$ and $q$ non-zero as the three parameter model. There is also a five parameter model which has hopping off on the left with rate $\gamma$ and on on the right with rate $\delta$ which we do not directly address in this paper.

The paper by Derrida et al \cite{1} originally found three different representations for the two parameter case. Representations of the three parameter model can be found in \cite{4} (and references therein) and for the five parameter model in \cite{5} (and references therein).

If the matrices associated with a given representation have sufficiently simple structure (e.g. bi- or tri-diagonal) then they can be usefully interpreted as transfer matrices for lattice path models \cite{6}. This leads to combinatorial methods for computing the inner product.

Each matrix representation is associated with a basis for the vector space upon which the matrices act. A very well known basis is the set $| n \rangle, n \geq 0$, generated by the action of $e^n$ on a vacuum vector $| 0 \rangle$ defined by $d | 0 \rangle = 0$. For the three parameter model this basis and its dual give a representation in which the components of the boundary vectors are related to $q$-binomial coefficients and the tri-diagonal matrix $d + e$ gives a three term recurrence related to $q$-Hermite polynomials \cite{5}.

The primary objective of this paper is the basis associated with the three parameter model representation obtained by Sasamoto \cite{4} where the tri-diagonal matrix $d + e$ gives a three term recurrence related to the Al-Salam–Chihara polynomials \cite{7}. We show that this basis is associated with a pair of distinct sequences, $\{P_n\}$ and $\{Q_n\}$, of polynomials. The polynomials $Q_n$ generate the basis when acting on the boundary vector $| V \rangle$ and the orthogonal dual vectors are generated by the polynomials $P_n$ acting on the dual boundary vector $\langle W \rangle$. Thus the basis is the set of vectors $| V_n \rangle = Q_n | V \rangle$ and the orthogonal dual basis set is $\langle W_n \rangle = \langle W \rangle P_n$. Since the
basis is generated by the boundary vector \( |V\rangle \) and its dual \( \langle W| \) we will refer to this as the ‘boundary basis’.

We show the two polynomial sequences are bi-orthogonal with respect to a certain linear functional \( L \), that is \( L(P_n Q_m) = \Lambda_n \delta_{n,m} \), where \( \Lambda_n \) is a scalar. For convenience the pair \( \{P_n\} \) and \( \{Q_m\} \) will be referred to as a bi-orthogonal pair of polynomial sequences, or BiOPS.

The uniqueness and existence of the BiOPS arises from the determinant of the bi-moment matrix whose elements are given by \( B_{nm} \). These elements satisfy a pair of \( q \)-recurrence relations. Unlike traditional orthogonal polynomials defined by Favard’s theorem (see [8] or [9]) (i.e. they satisfy a three-term recurrence relation), the BiOPS satisfy first order (uncoupled) \( q \)-recurrence relations. We show that the BiOPS are intimately associated with the decomposition of the bi-moment matrix into upper and lower triangular matrices. In fact the polynomial coefficients, when written in their own basis, are the matrix elements of the lower (for \( P_n \)) and upper (for \( Q_n \)) matrices—see equation (3.23).

2. The algebra

In this section we set up the tensor algebra used to represent the ASEP [10]. Let \( \mathcal{R} \) be the ring of integer coefficient commutative polynomials, \( \mathcal{Z}[\alpha, \beta, q] \) and \( \mathcal{M} \) the \( \mathcal{R} \)-module

\[
\mathcal{M} = \bigoplus_{n \geq 0} V_{2^n},
\]

where \( V_2 \) is a free rank two \( \mathcal{R} \)-module with generators \( d, e \). Here \( V^0 \) denotes the ring \( \mathcal{R} \) of the module and \( V_{2^n} = V_2 \otimes V_2 \otimes \cdots \otimes V_2 \) (\( n \) factors).

The homogeneous submodule \( V_{2^n} \), of degree \( n \), is generated by the standard monomial basis elements \( e_i \otimes e_i \cdots \otimes e_i \) where \( e_i \in \{d, e\} \). For brevity we will frequently omit the tensor product symbol, thus \( d_{emn} \) denotes \( d_{emn} \otimes \cdots \otimes e_{emn} \) etc.

We use the three parameter version of the original matrix Ansatz algebra equations of Derrida et al [1] as modified in [11]. The latter form allows for arbitrary monomial pre- and post-factors (\( u \) and \( v \) in the equations below). The original algebra was stated in terms of matrices and vectors. Here we give a slightly more abstract version by using a linear functional and use the shifted variables \( d \) and \( e \) rather than \( D \) and \( E \).

**Definition 1.** Let \( u, v \) be any monomial basis elements of \( \mathcal{M} \). The \( \mathcal{R} \)-module homomorphism \( L : \mathcal{M} \rightarrow \mathcal{R} \) is defined by the following equations:

\[
L(u \otimes (d \otimes e - q e \otimes d - q') \otimes v) = 0, \quad (2.2a)
\]

\[
L(u \otimes (d - b)) = 0, \quad (2.2b)
\]

\[
L((e - a) \otimes v) = 0, \quad (2.2c)
\]

where \( a = q'/\alpha - 1, \ b = q'/\beta - 1 \), with \( L(1) = 1 \) and extended linearly to other elements of \( \mathcal{M} \).

The reasons for the slightly more abstract linear functional formulation are as follows. The primary reason is because this is how traditional three-term recurrence polynomial orthogonality can be formulated (see Favard’s theorem [8]). This in turn allows for a direct combinatorial construction of orthogonality [12] without going via any integral representations. It also allows for other representations of the linear functional such as via double integral measures [13] or via inner products as was done in the original Derrida et al paper [1].
The matrix product Ansatz of [1] for the stationary state can now be (trivially) restated using the linear functional \( \mathcal{L} \).

**Theorem 1.** (Derrida, Evans, Hakin and Pasquier [1].) The stationary state probability distribution, \( f(\tau) \), of the two parameter ASEP for the system in state \( \tau = (\tau_1, \ldots, \tau_L) \), is given by

\[
f(\tau) = \frac{1}{Z_L} \mathcal{L} \left( \prod_{i=1}^{L} (\tau_i d + (1 - \tau_i) e) \right),
\]

where

\[
Z_L = \mathcal{L} \left( (d + e)^L \right)
\]

and \( \tau_i = 1 \) if site \( i \) is occupied and zero otherwise.

3. Bi-orthogonal pair of polynomial sequences

Consider the pair of sequences

\[
\{ P_n(d) \}_{n \geq 0}, \quad \{ Q_n(e) \}_{n \geq 0}
\]

of monic polynomials (where \( P_n \) and \( Q_n \) are degree \( n \)). We wish to determine if it is possible to find such a pair which are orthogonal with respect to \( \mathcal{L} \). In particular, do there exist such sequences for which \( \mathcal{L}(P_n Q_m) = \Lambda_n \delta_{n,m} \) with \( \Lambda_n > 0 \)? These two sequences will then give us a basis and a dual basis for the representation associated with the Al-Salam–Chihara polynomials obtained in [4, 5].

In order to show such a pair of sequences do indeed exist we consider the infinite dimensional ‘bi-moment matrix’, \( B \), whose matrix elements are given by

\[
B_{n,m} = \mathcal{L}(d^n e^m), \quad n, m \geq 0.
\]

Note, all matrices have rows and columns that are indexed by non-negative integers.

The bi-moment matrix elements satisfy a pair of partial difference equations as given in the following theorem.

**Theorem 2.** The bi-moment matrix elements, (3.2), satisfy the recursions

\[
B_{i,j} = (1 - q^j)B_{i-1,j-1} + aqB_{i,j-1}, \quad (3.3a)
\]

\[
B_{i,j} = (1 - q^i)B_{i-1,j-1} + bqB_{i-1,j}, \quad (3.3b)
\]

\( i, j > 0 \) with boundary values \( B_{0,j} = a^i \) and \( B_{i,0} = b^j \), \( i, j \geq 0 \).

Thus the matrix looks like

\[
B = \begin{pmatrix}
1 & a & a^2 & \cdots \\
b & 1 + h_0 q & a(1 + h_0 q^2) & \cdots \\
h^2 & b(1 + h_0 q^2) & 1 + h_0 q(1 + q + h_1 q^2) & \cdots \\
\vdots & \vdots & \vdots & \ddots \\
\end{pmatrix}
\]

where \( h_n = abq^n - 1 \).
Proof. The idea of the proof is to repeatedly use the commutator \( [e, d] = qe - qd = q' \) from (2.2a) to move an \( e \) (resp. \( d \)) to the left (resp. right). Thus
\[
d^n e^m = d^{n-1}(de)^{m-1},
\]
\[
d^n e^m = d^{n-1}(q' + qe)d^{m-1},
\]
\[
d^n e^m = q'd^{n-1}e^{m-1} + qd^{n-1}ede^{m-1}
\]
and
\[
d^{n-1}ede^{m-1} = q'd^{n-1}e^{m-1} + qd^{n-2}ed^{2}e^{m-1}.
\]
Commuting the lone \( e \) to the left gives
\[
d^{n-1}ede^{m-1} = \left(1 - q\right) \sum_{k=1}^{n-1} q^{k-1}d^{n-1}e^{m-1} + qd^{n-1}ed^{n-1}e^{m-1}
\]
and since the sum telescopes the result is
\[
d^n e^m = (1 - q^n)d^{n-1}e^{m-1} + q^nede^{m-1}.
\]
Using (2.2c) gives (3.3a). Similarly for (3.3b) \( \square \)

As will be shown below, the existence of the BiOPS requires that the determinant of the \((n + 1) \times (n + 1)\) sub-matrix
\[
B^{(n)} = \left(B_{i,j}\right)_{0 \leq i,j \leq n}
\]
be non-zero for all \( n \geq 0 \). Thus we require the following theorem.

**Theorem 3.** Let \( B^{(n)} = \left(B_{i,j}\right)_{0 \leq i,j \leq n} \) be the truncated \((n + 1) \times (n + 1)\) bi-moment matrix whose elements are defined by theorem 2. Then
\[
\det B^{(n)} = \prod_{i=1}^{n} \left(1 - q^{n+1-i}(1 - abq^{i-1})^{n+1-i}\right). \tag{3.10}
\]
The value of the determinant is a simple consequence of the LDU-decomposition of the bi-moment matrix as given by the following theorem.

**Theorem 4.** The LDU-factorization of the bi-moment matrix is
\[
B = LDLU, \tag{3.11}
\]
where the three matrices have elements determined by the following q-recurrences. The lower triangular matrix elements satisfy
\[
L_{i,j} = L_{i-1,j-1} + bq^{i}L_{i-1,j} \tag{3.12a}
\]
with \( L_{i,0} = b^i \) and \( L_{0,j} = \delta_{0,j} \). The upper triangular matrix elements satisfy
\[
U_{i,j} = U_{i-1,j-1} + aq^{i}U_{i,j-1} \tag{3.12b}
\]
with \( U_{i,0} = a^i \) and \( U_{0,j} = \delta_{0,j} \) and the diagonal matrix elements satisfy
\[
D_{i} = \left(1 - abq^{i-1}\right)\left(1 - q^{i}\right)D_{i-1} \tag{3.12c}
\]
with \( D_{0} = 1 \).
The proof of the theorem is detailed in section 5. The LDU-decomposition of the bi-
moment matrix is at the centre of the whole calculation. Once the decomposition is obtained
most of the other results are straightforward consequences. For the case of \( q = 0 \) the LDU-
decomposition and determinant in the \( D \) and \( E \) variables has been obtained by Krattenthaler [14].

We now use the bi-moment matrix to show the existence and uniqueness of the BiOPS. For \( n, m \geq 0 \) require the bi-orthogonality condition
\[
\mathcal{L} \left( P_n(d)Q_m(e) \right) = \Lambda_n \delta_{n,m},
\]
where \( \Lambda_n \) is a sequence of non-zero normalization factors determined by \( \mathcal{L} \) and the monic constraint.

If this bi-orthogonality is translated into the inner product form of the original matrix product Ansatz, then the equation is asking the question: does there exist polynomials \( P_n(d) \) and \( Q_m(e) \) in the matrices \( d \) and \( e \) such that
\[
\langle W | P_n(d)Q_m(e) | V \rangle = \Lambda_n \delta_{n,m}
\]
for vector \( |V\rangle \) and dual vector \( \langle W | \) defined by
\[
(d - b1)|V\rangle = 0
\]
and
\[
\langle W|(e - a1) = 0.
\]
If so we get sequences of basis vectors \( |\hat{V}_n\rangle \) and their orthonormal (with respect to \( \mathcal{L} \)) duals \( \langle \hat{W}_n | \) given by
\[
\langle \hat{W}_n | = \langle W | P_n(d) \frac{1}{\sqrt{\Lambda_n}} \quad \text{and} \quad | \hat{V}_n \rangle = \frac{1}{\sqrt{\Lambda_n}} Q_n(e) | V \rangle,
\]
where \( |\hat{V}_0\rangle = |V\rangle \) and \( \langle \hat{W}_0 | = \langle W |. \) We normalize so that \( \langle W | V \rangle = 1. \) From these sequences, and since the identity matrix is \( I = \sum_{n \geq 0} |\hat{V}_n \rangle \langle \hat{W}_n |, \) we get matrix representations of \( d \) and \( e \) via
\[
d_{n,m} = \langle \hat{W}_n | d | \hat{V}_m \rangle \quad \text{and} \quad e_{n,m} = \langle \hat{W}_n | e | \hat{V}_m \rangle
\]
which satisfy (2.2a).

This procedure for constructing basis vectors (see for example [3]) is analogous to the quantum oscillator basis set \( |n\rangle_{h \geq 0} \) constructed by the action of \( e^n \) on a vacuum vector \( |0\rangle \) which is defined by \( d |0\rangle = 0, \) that is, \( |n\rangle = e^n |0\rangle. \) The dual vectors are given via the action of \( d^n \) on the dual vacuum \( |0\rangle, \) that is \( \langle n| \prod_{n' = 1} (1 - q^n) = \langle 0 | d^n. \) In the BiOPS case the boundary vector \( |V\rangle \) plays the role of the vacuum vector and the basis set \( |\hat{V}_n\rangle_{h \geq 0} \) is generated by the action of \( Q_n(e) \neq e^n \) on \( |V\rangle \) defined by \( (d - b1)|V\rangle = 0. \) The dual vectors \( \langle \hat{W}_n | \) are similarly related to the action of \( P_n(d) \) on the dual boundary vector \( \langle W |. \)

Returning to the question of the existence of bi-orthogonal polynomials we have the following theorem stating a unique pair of sequences exists.

**Theorem 5.** Let \( \{P_n(d)\}_{h \geq 0} \) and \( \{Q_n(e)\}_{h \geq 0} \) be a pair of sequences of monic polynomials satisfying
\[
\mathcal{L} \left( P_nQ_m \right) = \Lambda_n \delta_{n,m},
\]
where the linear functional \( \mathcal{L} \) is defined by equation (2.2). Then \( \{P_n\}_{h \geq 0} \) and \( \{Q_n\}_{h \geq 0} \) exist and are unique with
\[ A_n = \prod_{i=1}^{n} \left( 1 - abq^{i-1} \right) \left( 1 - q^i \right) \]  
(3.18)

for \( n > 0 \) and \( A_0 = 1 \).

**Proof.** The existence of \( \{ P_n \} \) follows by applying Cramer’s rule to the system of linear equations obtained by writing

\[ P_n(d) = \sum_{k=0}^{n} a_k^{(n)} d^k \]  
(3.19)

with \( a_n^{(n)} = 1 \) and for \( k \leq n \),

\[ \mathcal{L}(P) = A_n B_{n,k} \]  
(3.20)

Since \( e^k = Q_k(e) + \sum_{\ell=0}^{k-1} e^\ell \mathcal{C}_\ell(e) \) and using equations (3.2) and (3.13) we get the system of equations

\[
\begin{pmatrix}
    a_0^{(n)}, a_1^{(n)}, \ldots, a_n^{(n)}
\end{pmatrix}
\begin{pmatrix}
    B_{0,0} & B_{0,1} & \cdots & B_{0,n} \\
    B_{1,0} & B_{1,1} & \cdots & B_{1,n} \\
    \vdots & \vdots & \ddots & \vdots \\
    B_{n,0} & B_{n,1} & \cdots & B_{n,n}
\end{pmatrix}
= \begin{pmatrix} 0, \ldots, 0, A_n \end{pmatrix}.
\]  
(3.21)

Since for all \( n \geq 0 \) we have from theorem 3 that \( \det B^{(n)} \neq 0 \) and thus the system has a unique solution given by Cramer’s rule

\[ P_n(d) = \frac{1}{\det B^{(n-1)}} \det 
\begin{pmatrix}
    B_{0,0} & B_{0,1} & \cdots & B_{0,n-1} & 1 \\
    B_{1,0} & B_{1,1} & \cdots & B_{1,n-1} & d \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    B_{n-1,0} & B_{n-1,1} & \cdots & B_{n-1,n-1} & d^{n-1} \\
    B_{n,0} & B_{n,1} & \cdots & B_{n,n-1} & d^n
\end{pmatrix} \]  
(3.22a)

Similarly

\[ Q_n(e) = \frac{1}{\det B^{(n-1)}} \det 
\begin{pmatrix}
    B_{0,0} & B_{0,1} & \cdots & B_{0,n-1} & B_{0,n} \\
    B_{1,0} & B_{1,1} & \cdots & B_{1,n-1} & B_{1,n} \\
    \vdots & \vdots & \ddots & \vdots & \vdots \\
    B_{n-1,0} & B_{n-1,1} & \cdots & B_{n-1,n-1} & B_{n-1,n} \\
    1 & e & \cdots & e^{n-1} & e^n
\end{pmatrix} \]  
(3.22b)

The scalar \( A_n \) follows from the monic requirement which gives

\[ A_n = \det B^{(n)}/\det B^{(n-1)}. \]

and hence from (3.10) we get (3.18). \[ \square \]

To find the explicit form of the polynomials we need to evaluate the two determinants (3.22a) and (3.22b). This requires the LDU-decomposition of the two matrices leading to the following lemma.

**Theorem 6.** The pair of sequences of monic polynomials \( \{ P_n(d) \}_{n \geq 0} \) and \( \{ Q_n(e) \}_{n \geq 0} \) satisfy the recurrence relations
\[ P_n(d) = d^n - \sum_{k=0}^{n-1} L_{n,k} P_k(d), \quad (3.23a) \]

\[ Q_n(e) = e^n - \sum_{k=0}^{n-1} Q_k(e) U_{k,n}, \quad (3.23b) \]

where \( L_{n,k} \) and \( U_{k,n} \) are the matrix elements of the lower triangular \( L \) and upper triangular \( U \) are given by (3.12).

**Proof.** The theorem follows from the LDU-decomposition (detailed in section 5) of the bi-moment matrix. This decomposition reduces (3.22) to the single determinant forms

\[
P_n(d) = \det \begin{pmatrix}
L_{0,0} & 0 & \ldots & 0 & 1 \\
L_{1,0} & L_{1,1} & \ldots & 0 & d \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
L_{n-1,0} & L_{n-1,1} & \ldots & L_{n-1,n-1} & d^{n-1} \\
L_{n,0} & L_{n,1} & \ldots & L_{n,n-1} & d^n
\end{pmatrix}, \quad (3.24a)
\]

and

\[
Q_n(e) = \det \begin{pmatrix}
0 & U_{0,1} & \ldots & U_{0,n-1} & U_{0,n} \\
1 & 0 & \ldots & U_{1,n-1} & U_{1,n} \\
0 & 0 & \ldots & U_{n-1,n-1} & U_{n-1,n} \\
1 & e & \ldots & e^{n-1} & e^n
\end{pmatrix}, \quad (3.24b)
\]

Expanding (3.24a) using the bottom row leaves a sub-matrix determinant which reduces down to a \( k \times k \) determinant of the same form as (3.24a) but with \( n = k \) and hence is \( P_k(d) \). Thus we get (3.23a). Similarly for (3.23b). \( \square \)

We now use (3.24a) to find explicit forms for \( P_n \) and \( Q_n \).

**Theorem 7.** The pair of sequences of monic polynomials \( \{P_n(d)\}_{n \geq 0} \) and \( \{Q_n(e)\}_{n \geq 0} \) are given by

\[
P_n(d) = \prod_{k=1}^{n} \left( d - bq^{k-1} \right)
\]

and

\[
Q_n(e) = \prod_{k=1}^{n} \left( e - aq^{k-1} \right)
\]

with \( P_0 = Q_0 = 1 \).
Proof. The theorem is equivalent to \( P_n \) and \( Q_n \) satisfying the first order recurrence relations

\[
P_{n+1}(d) = (d - bq^n)P_n, \quad (3.25a)
\]
\[
Q_{n+1}(e) = (e - aq^n)Q_n. \quad (3.25b)
\]

which we prove by induction using the recurrence relations (3.12) satisfied by the upper and lower triangular matrix elements. From theorem 6 we get

\[
dP_n = d^{n+1} - \sum_{k=0}^{n-1} L_{n,k} dP_k. \quad (3.26)
\]

The induction assumption is

\[
dP_{n-1} = P_n + bq^{n-1}P_{n-1}. \quad (3.27)
\]

Using (3.27) and (3.26) gives

\[
dP_n = d^{n+1} - \sum_{k=0}^{n-1} L_{n,k} (P_{k+1} + bq^k P_k). \quad (3.28)
\]

From theorem 6 we have

\[
P_{n+1} = d^{n+1} - \sum_{k=0}^{n} L_{n+1,k} P_k
\]

and using the recurrence relation for \( L \) from theorem 4 gives

\[
P_{n+1} = d^{n+1} - \sum_{k=0}^{n-1} L_{n,k} (P_{k+1} + bq^k P_k) - bq^n L_{n,n} P_n.
\]

Using (3.28) and since \( L_{n,n} = 1 \) we get

\[
P_{n+1} = dP_n - bq^n P_n.
\]

Since \( n = 1 \) is true, by induction, we have shown (3.25a). A similar induction proof gives (3.25b).

\[\square\]

4. Matrix representation in boundary basis

In this section we briefly discuss a representation of the linear functional \( \mathcal{L} \) by an inner product using a matrix representation of the tensor algebra.

The polynomials \( Q_n(e) \) generate a basis set \( \{v_n\}_{n \geq 0} \) for the module (2.1) by their action on the boundary monomial element \( v_0 \) satisfying \( \mathcal{L}(u(d - b)v_0) = 0 \), that is, generated by the set of elements \( v_n = Q_n(e)v_0 \). Denote the module in this basis by \( V_Q \). Note, equation (2.2b) shows that in the tensor space \( v_0 = 1 \) but is usually denoted \( |V_0 \rangle \) when \( \mathcal{L} \) is represented by an inner product.

It is well known that since \( V_Q \) is infinite dimensional that its dual space is not spanned by the elements, \( v_n^* \) dual to \( v_n \) (i.e. \( v_n^*(v_m) = \delta_{n,m} \)). Thus it is not clear a priori that all linear functionals \( \mathcal{L} \) that satisfy (2.2) can be expressed as an element in the dual sub-module spanned by \( v_n^* \). However, for the computational purposes of the ASEP model we only require a non-trivial such linear functional. It turns out to be sufficient to restrict ourselves to linear functionals in the dual sub-module spanned by \( v_n^* \). Call this dual sub-module \( V_{P_n}^* \). Thus we seek a linear functional \( \mathcal{L} \) satisfying (2.2) that exists in the dual sub-module \( V_{P_n}^* \).
Theorem 5 tells us that given the set \( \{v_n\} \) there exists a unique dual set \( v_n^* = P_n(d) \). We first find a matrix representation of the quotient module

\[
S = \mathcal{M}(de - q ed - q')
\]

and then address the question of how to extract \( \mathcal{L}(g) \), \( g \in S \), from the matrix representation of \( g \).

In order to obtain a matrix representation we need to use normalized sequences \( \{\hat{P}_n\}, \{\hat{Q}_n\} \) of the two polynomials sequences. If (3.13) is replaced by

\[
\mathcal{L}\left(\hat{P}_n \hat{Q}_m\right) = \delta_{n,m},
\]

then clearly

\[
\hat{P}_n = P_n/\sqrt{\Lambda_n}, \quad (4.3a)
\]

\[
\hat{Q}_n = Q_n/\sqrt{\Lambda_n} \quad (4.3b)
\]

gives a bi-orthonormal pair of polynomial sequences.

The recurrence relations (3.25) for \( P_n \) and \( Q_n \) can be used to compute the following two moments which lead to a matrix representation.

**Theorem 8.** Let \( P_n \) and \( Q_n \) be the polynomials of theorem 7. The two first moments

\[
X_{n,m} = \mathcal{L}(P_n d Q_m), \quad (4.4a)
\]

\[
Y_{n,m} = \mathcal{L}(P_n e Q_m), \quad (4.4b)
\]

for \( n, m \geq 0 \), are given by

\[
X_{n,m} = \Lambda_{n+1} \delta_{n+1,m} + bq^n \Lambda_n \delta_{n,m}, \quad (4.5a)
\]

\[
Y_{n,m} = \Lambda_{m+1} \delta_{n,m+1} + aq^m \Lambda_m \delta_{n,m}, \quad (4.5b)
\]

for \( n, m \geq 0 \).

The orthonormal versions of the polynomials give rise to a representation of the quotient module (4.1).

**Theorem 9.** The infinite dimensional matrices \( d \) and \( e \) with matrix elements

\[
d_{n,m} = \mathcal{L}\left(\hat{P}_n d \hat{Q}_m\right) = X_{n,m}/\sqrt{\Lambda_n \Lambda_m}, \quad (4.6a)
\]

\[
e_{n,m} = \mathcal{L}\left(\hat{P}_n e \hat{Q}_m\right) = Y_{n,m}/\sqrt{\Lambda_n \Lambda_m}, \quad (4.6b)
\]

for \( n, m \geq 0 \), give a matrix representation of the quotient module (4.1).

The theorem is proved by direct verification that the matrices (4.6) satisfy the quotient relation \( de - q ed = q'1 \).
The matrices (4.6) have a simple bi-diagonal structure
\[
d = \begin{pmatrix}
    b & \sqrt{c_0} & 0 & \cdots \\
    0 & bq & \sqrt{c_1} & \cdots \\
    0 & 0 & bq^2 & \cdots \\
    \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\] (4.7a)
and
\[
e = \begin{pmatrix}
    a & 0 & 0 & \cdots \\
    \sqrt{c_0} & aq & 0 & \cdots \\
    0 & \sqrt{c_1} & aq^2 & \cdots \\
    \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\] (4.7b)
where \(c_n = (1 - q^{n+1})(1 - abq^n)\). These are the same matrices obtained by Sasamoto [4].

The following theorem states the relationship between \(\mathcal{L}\) and the matrix representation.

**Theorem 10.** Let \(m\) be the matrix representation of an element \(m\) in the quotient module (4.1). Then
\[
\mathcal{L}(m) = m_{0,0},
\] (4.8)
where \(m_{0,0}\) is the \((0,0)\) matrix element of \(m\).

Equation (4.8) is the matrix product representation of \(\mathcal{L}\) conventionally written
\[
\mathcal{L}(e_e e_2 \cdots e_k) = \langle W | e_e e_2 \cdots e_k | V \rangle,
\] (4.9)
where \(e_i \in \{d, e\}\). In the basis \(|V_0\rangle\) we have
\[
\langle W | = \langle W_0 | = (1, 0, \ldots) \quad \text{and} \quad |V | = | V_0 \rangle = (1, 0, \ldots)^T.
\] (4.10)
Were \(T\) denotes the transpose.

**Proof.** Proof of theorem 10. Clearly (4.8) defines a linear functional from the space of matrices to \(R\). It remains to verify that such a functional satisfies the equation (2.2). Equation (2.2a) is satisfied as \(de - q \, ed - q \, 1\) is the zero matrix. Equation (2.2b) requires \(\mathcal{L}(u(d - b)) = u(d - b)_{0,0} = 0\) for any \(u \in S\), which trivially verified using the matrix (4.7a). Similarly for (2.2c).

Since the matrices \(d\) and \(e\) are upper and lower bi-diagonal respectively, their sum is clearly tri-diagonal and hence related to traditional three term recurrence orthogonal polynomials. In this case the tri-diagonal matrix is
\[
W_{n,m} = \mathcal{L}(\hat{P}_n(d + e)\hat{Q}_m) = \frac{X_{n,m} + Y_{n,m}}{\sqrt{\lambda_n \lambda_m}}.
\]
Thus the three term recurrence relation of the polynomials \(\{T_n(x)\}_{n \geq 0}\), is
\[
W_{n-1,n}T_{n-1} + (W_{n,n} - x)T_n + W_{n,n+1}T_{n+1} = 0
\] (4.11)
with initial values \(T_0 = 1\) and \(T_{-1} = 0\). These are essentially the Al-Salam–Chihara polynomials [7].
In this section we derive the decomposition of the bi-moment matrix into a product of a lower triangular matrix $L$, a diagonal matrix $D$ and an upper triangular matrix $U$ as given in theorem 11. In order to do this we extend a theorem in [15] by extracting the upper and lower matrices.

We start with the definition of matrices whose elements are given by a recurrence relation as stated in [15]. We will refer to such a matrix as a recursively defined matrix.

**Definition 2.** Let $\alpha = (\alpha_i)_{i \geq 0}$, $\beta = (\beta_i)_{i \geq 0}$, $\gamma = (\gamma_i)_{i \geq 0}$, $\mu = (\mu_i)_{i \geq 0}$, $\nu = (\nu_i)_{i \geq 0}$, $\epsilon = (\epsilon_i)_{i \geq 0}$ and $\lambda = (\lambda_i)_{i \geq 0}$ be given sequences. Let

\[
\begin{align*}
\Phi(i, j) &= \epsilon_{i-1}\gamma_{j-1} + \nu_{i-1}\mu_{j-1} \quad \text{for } i, j \geq 1, \\
\Psi(i, j) &= \epsilon_{i-1}\lambda_{j-1} + \nu_{i-1} \quad \text{for } i \geq 1, j \geq 0, \\
\Omega(i, j) &= [\alpha_i - \Psi(i, 0)\alpha_{i-1}](\beta_j - \mu_{j-1}\beta_{j-1}) \quad \text{for } i, j \geq 1.
\end{align*}
\]

A recursively defined matrix, is a matrix $A = (a_{i,j})$ of order $n + 1$ defined by $a_{0,j} = \alpha_0\beta_j$, $a_{i,0} = \beta_0\alpha_i$ for $0 \leq i, j \leq n$ and

\[
a_{i,j} = \mu_{j-1}a_{i,j-1} + \Phi(i, j)a_{i-1,j-1} + \Psi(i, j)a_{i-1,j} + \Omega(i, j)
\]

for $1 \leq i, j \leq n$.

For matrices whose elements satisfy the above definition the following theorem gives the decomposition.

**Theorem 11.** The unique LDU-decomposition for a recursively defined matrix is

\[A = L \cdot D \cdot U,\]

where $L$ (resp. $U$) is a lower (resp. upper) triangular matrix with diagonal entries 1 and $D$ is a diagonal matrix. Also $L = (l_{i,j})_{0 \leq i,j \leq n}$, $l = (l_{i,j})_{0 \leq i,j \leq n}$ and $D^{(1)}$ is a diagonal matrix with diagonal entries $(D^{(1)}_{i,j})_{0 \leq i,j \leq n}$ such that

\[l = L \cdot D^{(1)},\]

and

\[D^{(1)}_i = \alpha_0 \prod_{k=1}^{i-1} \epsilon_k,\]

where $l_{i,0} = \alpha_i$, $l_{0,j} = \delta_{0,j}$ and

\[l_{i,j} = \epsilon_{i-1}l_{i-1,j-1} + \Psi(i, j)l_{i-1,j},\]

and where $U = (u_{i,j})_{0 \leq i,j \leq n}$, $u = (u_{i,j})_{0 \leq i,j \leq n}$ and $D^{(2)}$ is a diagonal matrix with diagonal entries $(D^{(2)}_{i,j})_{0 \leq i,j \leq n}$ such that

\[u = D^{(2)} \cdot U.\]
and

\[ D^{(2)}_j = \sum_{k=1}^{j} \left\{ \beta_{k-1} \left( \gamma_{k-1} + \mu_{k-1} \lambda_{k-2} \right) \prod_{r=0}^{k-2} \left( \lambda_{j-r-1} \right) \prod_{s=k+1}^{j} \left( \gamma_{s-1} + \mu_{s-1} \lambda_{j-1} \right) \right\} + \beta_j \prod_{r=0}^{j-1} \left( \lambda_{j-1} - \lambda_{j-1} \right) \]

with \( u_{0,j} = \beta_j \) and \( u_{i,0} = \delta_{i,0} \) and

\[ u_{i,j} = \mu_{j-1} u_{i,j-1} + \left( \gamma_{j-1} + \mu_{j-1} \lambda_{j-2} \right) u_{i,j-1} + \left( \lambda_{j-1} - \lambda_{j-2} \right) u_{i,j-1} \]

and the diagonal matrix \( D \) has diagonal elements \( D_i \) such that

\[ D_i = D^{(1)}_i D^{(2)}_i. \]

This is a modified version of the main theorem in [15]. There the theorem states the determinant of a recursively defined matrix and proves the result using a LU-decomposition. Theorem 11 converts the LU-decomposition from the proof into the unique LDU-decomposition.

**Proof.** Proof of theorem 4. From the recursion in (3.3a) we get that the bi-moment matrix is a recursive matrix with

\[ \mu_j = 0, \nu_i = 0, \epsilon_i = 1, \gamma_j = 1 - q^{i+1}, \lambda_j = bq^{i+1}, \alpha_i = b^i, \beta_j = a^j, \]

therefore by theorem 11 we get

\[ L_{i,j} = L_{i-1,j-1} + bq^i L_{i-1,j}, \]

where \( L_{0,0} = b^0 \) and \( L_{0,j} = \delta_{0,j} \) with

\[ D_j = \sum_{k=1}^{j+1} (ab)^{j-k} \prod_{r=0}^{k-2} (q^j - q^r) \prod_{s=k}^{j} (1 - q^s) \]

which can be shown to satisfy

\[ D_j = \left( 1 - abq^{j-1} \right) \left( 1 - q^j \right) D_{j-1}. \]

To get the upper triangular matrix, we will instead find the lower triangular matrix of the transpose of the bi-moment matrix. From the recursion in (3.3b), we get that the transpose of the bi-moment matrix is a recursive matrix with

\[ \mu_j = 0, \nu_i = 0, \epsilon_i = 1, \gamma_j = 1 - q^{i+1}, \lambda_j = aq^{i+1}, \alpha_i = a^i, \beta_j = b^j, \]

therefore by theorem 11

\[ U_{ij}^T = U_{i-1,j-1}^T + aq^i U_{i-1,j}^T, \]

where \( U_{0,j}^T = a^j \) and \( U_{i,0}^T = \delta_{i,0} \). Taking the transpose of this matrix gives the required result. \( \square \)

6. Concluding Remarks

We have shown that the representation associated with the Al-Salam–Chihara polynomials obtained by Sasamoto [4] is a matrix representation of the quotient module \( \mathcal{M}/(de - qed - q^2) \) with respect to a basis \( |\psi_0\rangle = Q_0 |V\rangle \) generated by the boundary vector
V) via the action of the polynomial sequence \( \{Q_n\} \). The vectors, \( \langle W \rangle = \langle W \rangle P_n, \) dual to \( \{V_n\} \) are generated by the dual boundary vector \( \langle W \rangle P_n, \) through the action of the polynomials \( \{P_n\} \). The two sequences \( \{P_n\} \) and \( \{Q_n\} \) are bi-orthogonal with respect to the linear functional \( \mathcal{L} \) defined by the equation (2.2), that is \( \mathcal{L}(P_n Q_m) = \delta_{n,m} \). Using the bi-moment matrix (3.2) we showed that the two bi-orthogonal sequences exist and are unique. Through the LDU-decomposition of the bi-moment matrix it is possible to find explicit forms for the bi-orthogonal sequences in the case of the three parameter model.

It would also be of interest to compute the five parameter versions of \( P_n \) and \( Q_n \) which would presumably be associated with the same Askey–Wilson polynomials [16] obtained in [5, 11]. Preliminary work shows the five parameter generalization of the two \( q \)-recurrence relations, (3.3), for the bi-moment matrix are straightforward to derive but that the LDU-decomposition of the resulting matrix is significantly more complicated.

Finally, what about the combinatorics of this formalism? The connection between classical orthogonal polynomials and the combinatorics of lattice paths is well established [12, 17] as is the combinatorics of the ASEP model [2]. Clearly the bi-diagonal structure of the \( d \) and \( e \) matrices connect to binomial lattice paths (aka. fully directed paths) and the tridiagonal matrix \( W_{PdeQ} \mathcal{L} = \delta_{n,m} \) to Motzkin paths. However, in this instance there is no Hankel matrix of moments—it is replaced by the bi-moment matrix.

Acknowledgments

We would like to thank the Australian Research Council (ARC) and the Centre of Excellence for Mathematics and Statistics of Complex Systems (MASCOS) for financial support. I would also like to thank the referees for their useful comments.

References

[1] Derrida B, Evans M, Hakim V and Pasquier V 1993 Exact solution of a 1d asymmetric exclusion model using a matrix formulation J. Phys. A: Math. Gen. 26 1493–1517
[2] Blythe R A and Evans M R 2007 Nonequilibrium steady states of matrix-product form: a solver’s guide J. Phys. A: Math. Gen. 40 333
[3] Alexandre L and Vincent P 2014 Bethe ansatz and Q-operator for the open ASEP J. Phys. A: Math. Theor. 47 295202
[4] Sasamoto T 1999 One-dimensional partially asymmetric simple exclusion process with open boundaries: orthogonal polynomials approach J. Phys. A: Math. Gen. 32 7109–31
[5] Uchiyama M, Sasamoto T and Wadati M 2004 Asymmetric simple exclusion process with open boundaries and Askey–Wilson polynomials J. Phys. A: Math. Gen. 37 4985
[6] Brak R and Essam J W 2004 Asymmetric exclusion model and weighted lattice paths J. Phys. A: Math. Gen. 37 4183–217
[7] Gasper G and Rahman M 1990 Basic Hypergeometric Series (Cambridge: Cambridge University Press)
[8] Favard J 1935 Sur les polynomes de Tchebicheff C. R. Acad. Sci. Paris 200 2052–3
[9] Ismail M 2005 Classical and Quantum Orthogonal Polynomials in One Variable (Encyclopedia of Mathematics and its Applications) (Cambridge: Cambridge University Press)
[10] Crampe N, Ragoucy E and Vanicat M 2014 Integrable approach to simple exclusion processes with boundaries, review and progress J. Stat. Mech. P11032
[11] Corteel S and Williams L K 2011 Tableaux combinatorics for the asymmetric simple exclusion process and Askey–Wilson polynomials Duke Math. J. 159 385–415
[12] Viennot G 1985 A combinatorial theory for general orthogonal polynomials with extensions and applications Lecture Notes Math. 1171 139–57
[13] Bertola M, Eynard B and Harnad J 2002 Duality, biorthogonal polynomials and multi-matrix models Commun. Math. Phys. 229 73–120
[14] Krattenthaler C 2002 Evaluations of some determinants of matrices related to the Pascal triangle
Seminaire Lotharingien de Combinatoire **47** B47g
[15] Moghaddamfar A R, Navid Salehy S and Nima Salehy S 2008 The determinants of matrices with
recursive entries Linear Algebr. Appl. **428** 2468–81
[16] Askey R 1975 Orthogonal Polynomials and Special Functions vol 21 (Philadelphia, PA: SIAM)
[17] Flajolet P 1980 Combinatorial aspects of continued fractions Discrete Math. **32** 125–61