Geometric reductions of ABS equations on an $n$-cube to discrete Painlevé systems*

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Received 27 July 2014, revised 22 September 2014
Accepted for publication 26 September 2014
Published 25 November 2014

Abstract

In this paper, we show how to relate $n$-dimensional cubes on which ABS equations hold to the symmetry groups of discrete Painlevé equations. We here focus on the reduction from the four-dimensional cube to the $q$-discrete third Painlevé equation, which is a dynamical system on a rational surface of type $A_5^{(1)}$ with the extended affine Weyl group $\tilde{W}(A_2 + A_1)^{(1)}$. We provide general theorems to show that this reduction also extends to other discrete Painlevé equations at least of type A.

Keywords: ABS equations, discrete Painlevé equations, geometric reduction
PACS numbers: 02.30.Ik, 02.20.Qs

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

1. Introduction

We present a geometric method to obtain discrete Painlevé equations from higher-dimensional integrable discrete systems. Geometrically, symmetry groups of discrete Painlevé equations are affine Weyl groups, orthogonal to the divisor class of their initial value space in the Picard lattice [20, 23]. Higher dimensional discrete integrable systems arise from an entirely different geometric point of view, namely as multi-dimensionally consistent quad-equations embedded on a hypercube (we refer to the $n$–dimensional hypercube as the $n$-cube) [1, 2, 18].

Previous studies in the literature have performed reductions of such equations via methods suited to specific examples [8–11, 13, 17, 21, 22]. In particular, the identification of the reduced system has been mainly achieved by comparing or transforming it to known

* This research was supported by an Australian Laureate Fellowship # FL 120100094 and grant # DP130100967 from the Australian Research Council.
forms of the discrete Painlevé equations. It has been shown for systems such as the KP hierarchy and UC hierarchy that reduction from a higher-dimensional setting is more natural [15, 24, 26, 27]. We demonstrate here that it is indeed also the case for the higher-dimensional quad-equations consistent on the cube by providing a general geometric construction.

Multi-dimensionally consistent equations, with copies of the same equation holding on each face of a 3-cube (a symmetric 3-cube), were classified by Adler et al [1]. This is often referred to as consistency around the cube property. The results can be naturally extended to a symmetric n-cube and are called ABS equations. Boll [4] extended ABS equations to asymmetric 3-cubes, where equations on different faces may differ [3, 6]. These results were further extended to four-dimensional cubes with the exception of asymmetric systems that incorporate \( H^6 \)-type equations [6].

In this work, we construct a four-dimensionally consistent system that does incorporate \( H^6 \)-type equations and show that the geometrical nature of the construction gives us naturally the symmetry of its periodically reduced systems, not limiting to only reductions on two-dimensional (2D) lattice. We show explicitly the relation of its reduced systems to the \( q \)-Painlevé equations on \( A^{(1)}_5 \)-surface of Sakai’s classification.

Our main idea comes from the identification of the orthogonal projection of an \( n \)-cube in \( \mathbb{R}^{n} \) with the Voronoi cell of the \( (n - 1) \)-dimensional root lattice of type \( A_{n-1} \). In particular, we describe the dynamics of multi-dimensionally consistent quad-equations\(^1\) on the \( n \)-cube in the cubic lattice, \( \mathbb{Z}^n \), by using the translations of Voronoi cells in the weight lattice of the extended affine Weyl group \( \tilde{W}(A^{(1)}_n) \). For conciseness, we state our main results here without providing details of the proofs. Details will be given in a subsequent paper.

This work is motivated by our previous findings [14], where quad-equations were observed on what is called the \( \omega \)-lattice, constructed from the \( \tau \)-function theory of the \( A^{(1)}_5 \)-surface \( q \)-Painlevé system. The present paper begins at the other end of the story with quad-equations on an \( n \)-cube. We travel the other way to show how to construct higher-dimensional integrable systems from which \( q \)-Painlevé systems and extensions can be obtained along with their full parameters.

The plan of the paper is as follows. In section\( 2 \), we state the main idea of the \( n \)-cube, the Voronoi cell of the root lattice \( A_{n-1} \) and the quad-equations on an \( n \)-cube in theorems\( 1 \) and\( 2 \). We give an explicit example for the case \( n = 3 \). We show how to obtain the symmetry of \((1, 1, 1)\)-periodically reduced quad-equations on a symmetric 3-cube. This information is then used in the next section as the part of construction of a system of quad-equations on an asymmetric 4-cube. In section\( 3 \), we construct an asymmetric system of consistent quad-equations on a 4-cube by fitting eight 3-cubes in a self-consistent way. In section\( 4 \), we show how to obtain \( A^{(1)}_5 \)-surface \( q \)-Painlevé system by imposing a \((1, 1, 1)\)-periodic condition along a symmetric 3-cube inside of the asymmetric 4-cube. We give also the subcase of the \((1, 1, 1)\)-periodic condition, namely the \((2,1)\) periodic reduction. The latter example shows that our geometric approach on a higher dimensional setting includes periodic-type reductions on a 2D lattice approach. Finally, the paper ends with a conclusion.

\section{The \( n \)-cube and the Voronoi cell of the root lattice \( A_{n-1} \)}

We first recall some notations and definitions needed to describe our results. The root lattice \( A_{n-1} \) is the \( \mathbb{Z} \)-span of the simple roots \( \rho_i = \varepsilon_i - \varepsilon_{i+1}, \ 1 \leq i \leq n - 1 \) of the root system of type\(^1\) We use the term quad-equation throughout the paper to describe partial difference equations that relate the values of the solution on the vertices of a quadrilateral.
$A_{n-1}$, the corresponding Weyl group is $\mathcal{W}(A_{n-1}) = \langle s_1, \ldots, s_{n-1} \rangle = \mathfrak{S}_n$, where $\mathfrak{S}_n$ denotes the symmetric group, which acts by permuting the $\epsilon_i$. The fundamental weights $h_i$, $1 \leq i \leq n - 1$, are defined by the inner product $(h_i, \rho_j) = \delta_{ij}$.

For systems of type $A_{n-1}$, the fundamental weights are defined by

$$h_k = (\epsilon_1 + \cdots + \epsilon_k) - \frac{k}{n} \sum_{i=1}^{n} \epsilon_i, \quad 1 \leq k \leq n - 1. \quad (2.1)$$

The weight lattice of type $A_{n-1}$ is the $\mathbb{Z}$-span of the fundamental weights $\rho$, $\rho_i$, $\leq \rho_j$, $\leq -\rho_i$, $\in 11$. The Voronoi cell $V(0)$ is the convex hull of

$$\{ w_S \} = \bigcup_{0 \leq k \leq n, w \in \mathfrak{S}_n} w(h_k). \quad (2.2)$$

where $S \subseteq \{1, \ldots, n\}$ and we have set $h_n = h_0 = w_0 = 0$. $V(0)$ tessellates $\mathcal{W}(A_{n-1})$ by translations $[7, 16]$. The highest root of the root system of type $A_{n-1}$ is

$$\rho = \sum_{i=1}^{n-1} \rho_j = h_1 + h_{n-1}, \quad (2.3)$$

where $\rho_i$ are the simple roots. The extended affine Weyl group $\widetilde{\mathcal{W}}(A^{(1)}_{n-1})$ has generators $\langle s_0, s_1, \ldots, s_{n-1}, \pi \rangle$, which satisfy the following relations

$$s_i^2 = 1, \quad (s_i s_{i+1})^3 = 1, \quad (i \in \mathbb{Z}/n\mathbb{Z}) \quad (2.4a)$$

$$\pi^n = 1, \quad \pi s_i = s_{i+1} \pi. \quad (2.4b)$$

The generators of the finite Weyl group $s_i$, $1 \leq i \leq n - 1$ act on $h_i$ to give the $\mathcal{W}$-orbit of $h_i$ and

$$s_i h_k = h_{k'}, j \neq k, \quad (2.4c)$$

and

$$\pi(h_k) = h_{k+1}, \quad (k \in \mathbb{Z}/n\mathbb{Z}). \quad (2.4d)$$

By definition $[12]$

$$s_0(v) = s_{\beta_1}(v) = v - (v, \rho) - 1)\rho, \quad v \in \mathbb{R}^n, \quad (2.4e)$$

therefore we have

$$s_0(h_k) = h_k \text{ for } k \neq 0, \quad \text{and} \quad s_0(h_0) = \rho = h_1 + h_{n-1}. \quad (2.4f)$$

The extended affine Weyl group can be represented as the semidirect product of the finite Weyl group and the translation group corresponding to the weight lattice $\widetilde{\mathcal{W}}(A^{(1)}_{n-1}) = \mathcal{W}(A_{n-1}) \ltimes P(A_{n-1})$. Let $T_j$, $1 \leq j \leq n$, denotes translation in the $j$th direction of the $n$-dimensional representation of $A_{n-1}$ in $\mathbb{R}^n$ [19]

$$T_i = \pi s_{n-1} \cdots s_1, \quad T_1 = s_{n-1} \pi \ldots s_1 \pi, \quad T_2 = s_{n-1} \pi \ldots s_2 \pi, \ldots, T_n = s_{n-1} \pi \ldots s_{n-1}, \quad T_n \ldots T_1 = 1. \quad (2.4h)$$

The $n$-cube is a combinatorial object, which can be embedded in $\mathbb{R}^n$ as follows: $x_S = \sum_{i \in S} \epsilon_i$, where $\epsilon_i$ are the unit vectors of $\mathbb{R}^n$ and $S \subset \{1, \ldots, n\}$. There is a unique vertex $\xi$, which is ‘furthest’ from $x_0$, being $n$ steps away: $\xi = \sum_{i=1}^{n} x_i$. The condition $\xi = x_0$ is
equivalent to the orthogonal projection ϕ of the n-cube w.r.t ξ

\[ \phi(x_\xi) = v - \frac{(x_\xi, \xi)}{\|\xi\|} \]  

(2.5)

**Theorem 1.** The convex hull of \( \phi(x_\xi), S \subseteq \{1, ..., n\}, \) is the Voronoi cell \( V(0) \) around the origin of \( A_{n-1} \) root lattice. That is, \( \phi(x_\xi) = w_S \).

**Theorem 2.** The system of quad-equations

\[ \frac{w_S + c_i}{w_S + c_j} = \frac{a_i w_S + a_j w_S + c_i + c_j}{a_i w_S + a_j w_S + c_i + c_j}, \quad S \subseteq \{1, ..., n\}, \quad i, j \not\in S, \quad 0 \leq |S| \leq n - 2, \]  

(2.6)

under the \((1,...,1)\) periodic condition

\[ T_n...T_1 w_S = w_S, \]  

(2.7)

is invariant under the symmetry group \( \tilde{W}(A^{(1)}_{n-1}) \), where \( S + c_i \) refers to a vertex on the n-cube, \( \{ w_S \} \) are the variables of the quad-equation, defined on the vertices of \( V(0) \). The system of quad-equations (2.6) are known as the \( H_{3:0} \) equation in the ABS classification. (For brevity we denote it here by \( H_3 \).) Furthermore, we have the following:

1. Let \( a_j = \frac{a_{j-1}}{a_j}, 1 \leq j \leq n - 1, \) and define \( a_0 = \frac{a_1}{a_0} \), so that \( a_0 a_1 ... a_n-1 = q \), where \( q \) is a constant. The reflection generators of the finite Weyl group \( s_i, 1 \leq i \leq n - 1, \) act on the variables of the quad-equations \( w_S \) by permuting the indices, and their actions on the parameters are defined as follows

\[ s_i(a_j) = a_j a_i^{A_{ij}}, \quad 1 \leq i, j \leq n - 1, \]  

(2.8)

where \( A_{ij} \) is the entry of the Cartan matrix of type \( A_{n-1} \)

\[ A = \left( A_{ij} \right)_{i,j=1}^{n-1} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & \ddots \\ 0 & \ddots & -1 \end{pmatrix}. \]

The actions of the translations on the parameters and the \( w_S \) variables are defined by

\[ T_j(w_S) = w_{S + c_j}, \quad T_j(a_i) = \begin{cases} \frac{a_i}{q}, & j = i, \\ qa_i, & j = i + 1, \\ a_i, & j \not= i, i + 1, \end{cases} \]  

(2.9)

where \( i, j \in \mathbb{Z}/n\mathbb{Z} \). This corresponds to the tessellation of \( \mathbb{R}^{n-1} \) by translations of \( V(0) \) in the weight lattice.

2. All of the \( 2^n \) \( w_S \) variables can be expressed in terms of the \( n \) initial values which correspond to the fundamental weights \( h_k, 0 \leq k \leq n - 1 \) defined in equations (2.1)–(2.2). The actions of the generators \( \pi \) and \( s_0 \) can be obtained from those of the finite reflections and translations. In particular, from equations (2.4g) and (2.8)–(2.9) we have

\[ \pi = T_1 s_1 ... s_{n-1}, \]  

(2.10)

and
\[ \pi(a_i) = a_{i+1}, \]
\[ \pi(h_k) = h_{k+1}, \quad k \in \mathbb{Z}/n\mathbb{Z}, \quad (2.11) \]

where action of \( \pi \) on the initial values \( h_k \) is given by equation (2.4d).

From equation (2.4f) we see that the action of \( s_0 \) on the initial values \( h_k, 1 \leq k \leq n - 1 \) are trivial except on \( h_0 \), whose action can be derived from equations (2.6) and (2.9)
\[ s_0(h_0) = h_0 \frac{h_{n-1} + h_1/a_0}{h_{n-1} + a_0h_1}. \quad (2.12) \]

Using the definition
\[ s_0 = \pi^{-1}s_1\pi, \quad (2.13) \]
we have
\[ s_0(a_{n-1}) = a_{n-1}a_0, \]
\[ s_0(a_0) = 1/a_0, \]
\[ s_0(a_1) = a_1a_0. \quad (2.14) \]

Theorems 1 and 2 provide a general method for constructing systems of multi-dimensionally consistent quadrilateral equations and simultaneously provide the symmetry groups of its periodic reductions on an \( n \)-cube. We call this method the ‘geometric reduction’ of such quad-equations on an \( n \)-cube. In the rest of this section we give an explicit application of theorems 1 and 2 in the case \( n = 3 \).

### 2.1. Symmetry of \((1, 1, 1)\) periodically reduced quad-equations on a symmetric 3-cube

For the case \( n = 3 \), \( x_{(1,2,3)} \) are the eight vertices of the 3-cube: \( x_0 = 0, x_1 = e_1, x_2 = e_2, x_3 = e_3, x_{12} = e_1 + e_2, x_{13} = e_1 + e_3, x_{23} = e_2 + e_3, x_{123} = e_1 + e_2 + e_3 = \xi \).

The extended affine Weyl group of type \( A_2 \) is \( \tilde{W}(A_2^{(1)}) = \langle s_0, s_1, s_2, \pi \rangle \), with the relations
\[ s_j^2 = 1, \quad (s_j s_{j+1})^3 = 1, \quad (j = 0, 1, 2), \quad (2.15a) \]
\[ \pi^3 = 1, \quad \pi s_j = s_{j+1} \pi, \quad (2.15b) \]
and translations \( T_i \) \( (i = 1, 2, 3) \)
\[ T_1 = \pi s_2 s_1, \quad T_2 = s_1 \pi s_2, \quad T_3 = s_2 s_1 \pi, \quad T_1 T_2 T_3 = 1. \quad (2.15c) \]

\( \tilde{W}(A_2^{(1)}) \) has a representation in \( \mathbb{R}^3 \) as follows: the simple roots \( \rho_1 = e_1 - e_2, \rho_2 = e_2 - e_3, \) and the highest root is \( \tilde{\rho} = e_1 - e_3 \). The two fundamental weights \( h_1 = w_1, h_2 = w_2 \). Their respective \( \mathcal{W} \)-orbits are:
\[ w_1 = \frac{1}{3}(2e_1 - e_2 - e_3), s_1(w_1) = w_2 = \frac{1}{3}(-e_1 + 2e_2 - e_3), \]
\[ s_2(w_1) = w_3 = \frac{1}{3}(-e_1 - e_2 + 2e_3), w_1 = \frac{1}{3}(e_1 + e_2 - 2e_3), \]
\[ s_1(w_2) = w_{12} = \frac{1}{3}(-e_1 - e_2 + 3e_3), s_2(w_{12}) = w_{23} = \frac{1}{3}(3e_1 - 2e_2 + e_3). \]

The orthogonal projection \( \phi \), equation (2.5) maps the 3-cube to the Voronoi cell of \( A_2 \),
\[ \phi(x_{(1,2,3)}) = w_{(1,2,3)}: \]
\[ \phi(x_1) = w_1, \quad \phi(x_2) = w_2, \quad \phi(x_3) = w_3, \]
\[ \phi(x_{12}) = w_{12}, \quad \phi(x_{13}) = w_{13}, \quad \phi(x_{23}) = w_{23}. \]
and $\phi(x_{123}) = w_{123} = w_0 = \phi(x_0)$. Thus the orthogonal projection of the 3-cube gives the $(1, 1, 1)$ ‘periodic condition’: $w_{123} = w_0$ of the quad-equations, which comes from the relation $T_1T_2T_3 = 1$ of $\mathcal{W}(A_2^{(1)})$.

The fundamental simplex of $A_2^{(1)}$ lattice is the convex hull of $w_0, w_1, w_{12}$, i.e. an equilateral triangle $F$ bounded by the reflections described by the reflection generators $\langle s_0, s_1, s_2 \rangle$, and $\pi$ acts by rotating anti-clockwise $120^\circ$ around the barycenter of $F$. We obtain the Voronoi cell at the origin $V(0)$ by applying reflections of $\mathcal{W}(A_2)$ to $F$, and we can cover the whole 2D plane by translating $V(0)$ [19]. $\mathcal{W}(A_2)$ is the symmetric group $\mathcal{S}_3 = \{1, s_1, s_2, s_1s_2, s_2s_1, s_1s_2s_1 = s_2s_1s_2\}$, that is $|\mathcal{S}_3| = 6$.

From

$$V(0) = \bigcup_{w \in \mathcal{S}_3} wF,$$  

we see that $V(0)$ is a hexagon made up of the union of six equilateral triangles. See figure 1.

The quad-equations on the 3-cube are the realizations of the reflections in $\mathcal{W}(A_2^{(1)})$

$$s_0(w_0) = w_{12} = \frac{w_0(qaw_1 + qw_{12})}{qw_1 + qaw_{12}},$$  

$s_1(w_1) = w_2 = \frac{w_1(\alpha w_0 + \beta w_{12})}{\beta w_0 + \alpha w_{12}},$  

$s_2(w_{12}) = w_1 = \frac{w_{12}(\beta w_1 + \gamma w_0)}{\gamma w_1 + \alpha w_0}$,  

where $w_1, w_{12}$ and $w_0$ are the three initial values of the system of quad-equations, corresponding to the fundamental weights $h_1, h_2$ and $h_0$. Define

$$a_1 = \frac{\beta}{\alpha}, \quad a_2 = \frac{\gamma}{\beta}, \quad a_0 = \frac{q\alpha}{\gamma}.$$  

Figure 1. Voronoi cell of $A_2^{(1)}$ lattice, a hexagon.
we have
\[ s_i(a_j) = a_j a_i^{-A_{ij}}, \quad 0 \leq i, j \leq 2, \] (2.21)
where \( A_{ij} \) is the entry of the Cartan matrix of type \( A_2^{(1)} \)
\[ A = (A_{ij})_{i,j = 0} = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \]
The actions of \( \pi \) are
\[ \pi(w_0) = w_1, \quad \pi(w_1) = w_{12}, \quad \pi(w_{12}) = w_0, \] (2.22)
\[ \pi(a_0) = a_1, \quad \pi(a_1) = a_2, \quad \pi(a_2) = a_0. \] (2.23)
Translations of \( \overrightarrow{W}(A_2^{(1)}) \) act on the vertices of the Voronoi cell by translating them in the directions along \( w_1, w_2 \) and \( w_3 \). For example
\[ T_1(w_0) = w_1, \]
\[ T_1(w_1) = w_{11}, \]
\[ T_1(w_{12}) = w_{112}. \] (2.24)
and actions on the parameters are
\[ T_1(a_1) = a_1/q, \quad T_2(a_1) = qa_1, \]
\[ T_2(a_2) = a_2/q, \quad T_3(a_2) = qa_2, \]
\[ T_3(a_0) = a_0/q, \quad T_1(a_0) = qa_0. \] (2.25)
We here see that the \((1, 1, 1)\) reduction of the symmetric 3-cube with \( H_3 \) equations results in a system with \( \overrightarrow{W}(A_2^{(1)}) \) symmetry. It is known that the full symmetry of the \( q \)-discrete Painlevé equation associated with surface type \( A_5^{(1)} \) has \( \overrightarrow{W}(A_2 + A_1)^{(1)} \) symmetry. In the next section we construct the higher dimensional system, in particular, quad-equations consistent on an asymmetric 4-cube. By reduction, this will give rise to exactly the \( q \)-discrete Painlevé equation with \( \overrightarrow{W}(A_2 + A_1)^{(1)} \) symmetry.

3. Equations on an asymmetric 4-cube
To construct a 4-cube, we need four lattice directions \( l, m, n, k \) and four lattice parameters \( \alpha(l), \beta(m), \gamma(n), \lambda(k) \). Let the dependent variable be \( x = x(l, m, n, k) \) and denote its shifts in each direction respectively by
\[ \hat{x} = x_1 = x(l + 1, m, n, k), \] (3.1a)
\[ \hat{x} = x_2 = x(l, m + 1, n, k), \] (3.1b)
\[ \hat{x} = x_3 = x(l, m, n + 1, k), \] (3.1c)
\[ \hat{x} = x_4 = x(l, m, n, k + 1). \] (3.1d)

3.1. Symmetric 3-cube \( C_{312} \)
We start with the \( H_3 \) quad-equation (3.2a) on a face of the 4-cube given by the \( l, n \) directions, where \( x = x(l, n), x_1 = x(l + 1, n), x_3 = x(l, n + 1), x_{13} = x(l + 1, n + 1) \). We construct a
symmetric system of equations (3.2a)-(3.2e) on a 3-cube by taking auto-Bäcklund transformations of equation (3.2a)

\[ Q(x, x_1, x_2, x_3; \alpha, \gamma) := xx_3 + x_1x_3 - \alpha/\gamma (xx_1 + x_3x_3) = 0, \quad (3.2a) \]

\[ Q(x, x_1, x_2, x_1; \alpha, \beta) = 0, \quad (3.2b) \]

\[ Q(x, x_3, x_2, x_2; \gamma, \beta) = 0, \quad (3.2c) \]

\[ Q(x_1, x_1, x_1, x_1; \gamma, \beta) = 0, \quad (3.2d) \]

\[ Q(x_2, x_1, x_3, x_1; \alpha, \gamma) = 0, \quad (3.2e) \]

where \( x_2 \) denotes the auto-Bäcklund transformation of \( x \) with Bäcklund parameter \( \beta \). We denote this 3-cube by \( C_{312} \). See figure 2(a).

In this system we have four initial values \( x, x_1, x_2, x_3 \); and three quad-equations (3.2a)-(3.2c), adjacent to the vertex \( x \). Vertices \( x_{12}, x_{13}, x_{23} \) are evaluated using the initial conditions and equations (3.2a)-(3.2c). \( x_{123} \) can then be evaluated using equations (3.2d) and

Figure 2. Two types of 3-cubes \( C_{312} \) and \( C_{134} \) with different arrangements of equations on faces.

Figure 3. The colours red, blue, green and yellow denote edges that are labelled by the same respective colours in figure 2.
3D consistency of the system means that $x_{123}$ evaluated by these three equations coincide. This is true in $n$-dimensions, i.e., it is multi-dimensionally consistent and hence it can be embedded on an $n$-cube. It is this remarkable fact we are going to utilize in deriving discrete Painlevé equations as periodic reductions on an $n$-cube. However, note that multidimensional consistent systems are not limited to systems with the same equation on all the faces.

3.2 Asymmetric 3-cube $C_{134}$

Now consider a non-auto Bäcklund transformation of (3.3) giving rise to different equations on different pairs of faces on the 3-cube. Here, we use equations from Boll’s classification of asymmetric 3-cubes [5] ((3.29)–(3.30) with $\delta_2 = \delta_3 = 0$). The 3-cube contains two $H_4$ type ($H_3$) equations on the ‘$Q$’ faces and four $H_6$ type equations for the ‘$A’ and ‘$C’ faces.

$$
Q(x, x_1, x_3, x_{13}; \alpha, \gamma) := xx_1 + x_3x_{13} - \alpha/\gamma (x_1 + x_3x_{13}) = 0,
$$

(3.3a)

$$
A(x, x_3, x_4, x_{34}; \delta_1) = xx_4 + x_3x_{34} + \delta_1xx_3 = 0,
$$

(3.3b)

$$
C(x, x_1, x_4, x_{14}; \delta_1\eta_1) = xx_4 + x_1x_{14} + \delta_1\eta_1xx_1 = 0,
$$

(3.3c)

$$
A' = A(x_1, x_3, x_{14}, x_{134}; \delta_1) = x_1x_{14} + x_3x_{134} + \delta_1x_1x_{13} = 0,
$$

(3.3d)

$$
C' = C(x_3, x_1, x_{34}, x_{134}; \delta_1\eta_1) = x_3x_{34} + x_1x_{134} + \delta_1\eta_1x_1x_{13} = 0,
$$

(3.3e)

$$
Q(x_4, x_{14}, x_{34}, x_{134}; \alpha, \gamma) = 0,
$$

(3.3f)

where $x_4$ denotes the non-auto Bäcklund transformation of $x$ and $\eta_1 = \alpha/\gamma$. The parameter $\delta_1$ initially is a function of $l, m, n$ and $k$, to be specified by the consistency conditions as we construct the 4-cube. Equations (3.3a)–(3.3f) make up the six quad-equations consistent on an asymmetric 3-cube. We denote this 3-cube by $C_{134}$, see figure 2(b).

Note that in obtaining equations (3.3a)–(3.3f) we have used

$$
\delta_1 = \delta_1', \quad \frac{\delta_1}{\gamma} = \frac{\alpha}{\gamma} = \frac{\delta_1'}{\gamma} 
$$

(3.4)

Each of the above constructions can be repeated to obtain two more 3-cubes labelled $C_{214}$ and $C_{324}$. $C_{214}$ is obtained in the same way as $C_{134}$ by replacing subscript 3 with 2 everywhere, with the condition $\eta_2 = \gamma/\beta$. $C_{324}$ is obtained from $C_{214}$ by replacing subscript 1 with 3 everywhere, with the condition $\eta_3 = \alpha/\beta$. In obtaining these two 3-cubes, we have imposed the following conditions

$$
\delta_2 = \delta_3 = \delta_1, \quad \frac{\delta_1}{\gamma} = \frac{\beta}{\gamma}
$$

(3.5)

Equations (3.4) and (3.5) imply that

$$
\delta_1(n, k) = \gamma(n)K(k),
$$

(3.6)

where $K$ is an arbitrary function of $k$.

We extend the above construction to four dimensions in the following way. The cube $C_{3124}$ is obtained by shifting $C_{312}$ in the $k$ direction, $C_{1342}$ by shifting $C_{134}$ in the $m$ direction, $C_{2143}$ by shifting $C_{214}$ in the $n$ direction and $C_{3241}$ by shifting $C_{324}$ in the $l$ direction. In summary, there are four 3-cubes adjacent to $x_{l234}$, namely $C_{3124}$, $C_{1342}$, $C_{2143}$ and $C_{3241}$. These four 3-cubes
are all 3D consistent under the conditions (3.4) and (3.5). Hence, we have eight three dimensionally consistent 3-cubes fitted consistently in a 4-cube. See figure 3(a).

The result contains two Bäcklund transformations, i.e., equations (3.2e) and (3.3f), of the equation on the bottom face of the 4-cube, namely equation (3.2a). The permutability of these two Bäcklund transformations provides a system of 24 quad-equations, which can be embedded consistently on the 24 faces of the 4-cube. By construction, the system of equations on this 4-cube is four dimensionally consistent [6].

3.3. A (1, 1, 1)-reduction on the asymmetric 4-cube

We apply a periodic condition on the asymmetric 4-cube

$$\hat{\beta} = -i\lambda x,$$  (3.7)

where $\hat{\beta}$ is only a function of $k$ and $\lambda = q\hat{\alpha}$. We call this a (1, 1, 1)-reduction of the 4-cube.

We have the following conditions on the lattice parameters in the $l, m, n$ directions:

$$\alpha = \alpha(l) = e^{i\gamma q}, \beta(m) = e^{\delta q^m}, \gamma(n) = e^{iq^n}.$$  

The periodic condition (3.7) enables us to evaluate $x(l, m, n, k)$ at any point in the lattice defined by the three directions $l, m, n$, using the initial conditions $x, x_1, x_2, x_3$ and the quad equations (3.2a)–(3.2c).

On the asymmetric 3-cube $C_{214}$, shaded pink in figure 3, we have six equations for its six faces

$$Q(x, x_1, x_2, x_{12}; \alpha, \beta) = 0,$$  (3.8a)

$$A(x, x_2, x_4, x_{24}; \delta) = xx_4 + x_2x_{24} + \delta_1 \beta \gamma^{-1} x_{x_2} = 0,$$  (3.8b)

$$C(x, x_1, x_4, x_{14}; \delta_3 \gamma^3) = xx_4 + x_1x_{14} + \delta_1 \alpha \gamma^{-1} x_{x_1} = 0,$$  (3.8c)

$$A' = A(x_1, x_2, x_{14}, x_{124}; \delta) = x_1x_{14} + x_{12}x_{24} + \delta_1 \beta \gamma^{-1} x_{x_1} = 0,$$  (3.8d)

$$C' = C(x_2, x_{12}, x_{24}, x_{124}; \delta_3 \gamma^3) = x_2x_{24} + x_{12}x_{124} + \delta_1 \alpha \gamma^{-1} x_{x_2} = 0,$$  (3.8e)

$$Q(x_4, x_{14}, x_{24}, x_{124}; \alpha, \beta) = 0.$$  (3.8f)

From (3.2b), (3.8b) and (3.8e), we find

$$\frac{x_{12}}{x} \frac{x_{24}}{x} = 1 \Rightarrow \frac{(\alpha x - \beta x_2)(x_{12} + \alpha K_{12})}{(\beta x_1 - \alpha x_2)(x_4 + \beta K_{24})} = 1.$$  (3.9)

(This follows from the tetrahedron property [1] and by ‘summing’ the three-leg forms of the equations on the faces adjacent to $x_{2}$.) Moreover, from the face shaded blue in figure 3(b) on which holds the equation for $x_{12}, x_{124}, x_{1234}$, and $x_{123}$ we have another expression for $x_{124}$

$$x_{124} = -\frac{x_{12}(x_{124} + \gamma K_{123})}{x_{123}} \Rightarrow -iq\hat{x}_4 = \frac{x_{12}(x_{124} - i\gamma K_{12})}{i\hat{x}},$$  (3.10)

where we have used the periodic condition (3.7) in rewriting the last equation. Using (3.10) to eliminate $x_{124}$ in (3.9), we finally have
4. Relation to $q$-Painlevé equations

In this section, we identify $q$-Painlevé equations from the $(1, 1, 1)$-reduction of the 4-cube described in section 4. Observing that the reduction collapses the 3-cubes $C_{312}$ and $C_{3124}$ in figure 3(b) to two copies of a hexagon, which can be extended everywhere in the triangular lattice, we find the affine Weyl group $\tilde{\mathcal{W}}(A_5^{(1)})$. But the fourth direction relating the two 3-cubes provides us with an extra direction that leads to a lattice with Affine Weyl symmetry group $\tilde{\mathcal{W}}((A_2 + A_1)^{(1)})$, which is the full symmetry group of the $A_5^{(1)}$-surface $q$-Painlevé equation. A sub-case of the $(1, 1, 1)$-reduction leads us to the symmetric version of this equation, which is often called the second $q$-discrete Painlevé equation ($q$-P$_{II}$).

Define

$$x(l, m, n, k) = (-1)^{l(m+n+k)} \lambda^{l+n+k} \omega(l, m, n, k),$$

then the periodic condition $\hat{\omega} = -i \lambda x$ implies

$$\hat{\omega} = \omega.$$ (4.2)

On letting $K = \lambda^{-1}(q\lambda^2 - 1)$, $\beta \alpha^{-1} = a_1$, $\gamma \alpha^{-1} = q^{-1}a_0$, and $\gamma \beta^{-1} = a_2$, our $q$-periodically reduced system on the asymmetric 4-cube is exactly the $\omega$-lattice constructed from the $\tau$-function framework of $A_5^{(1)}$-surface $q$-Painlevé system [14]. Results from [14] are reproduced in the appendix to show that iterations of $\omega$ in the $l$, $m$, $n$ and $k$ direction give rise to the affine Weyl group $\tilde{\mathcal{W}}((A_2 + A_1)^{(1)})$.

Figure 4 shows the vertices of the 4-cube now relabeled in $\omega$ variables. The quad-equations on the faces adjacent to $\omega$ are

$$\lambda \hat{\omega} = \alpha \omega - \beta \lambda \omega$$

$$\frac{\lambda \hat{\omega}}{\omega} = \frac{\alpha \omega - \beta \lambda \omega}{\omega}$$ (4.3a)

$$\gamma \hat{\omega} = \alpha \omega - \gamma \omega$$

$$\frac{\gamma \hat{\omega}}{\omega} = \frac{\alpha \omega - \gamma \omega}{\omega}$$ (4.3b)
The expression relating $\circ$, $\bar{\circ}$ and $\hat{\circ}$ directions is given by transforming equation (3.11) to $\omega$ variables

$$\frac{\lambda \hat{\omega}}{\omega} = \frac{\beta \lambda \hat{\omega} - \gamma \hat{\omega}}{-\gamma \lambda \hat{\omega} + \beta \hat{\omega}}$$  \hfill (4.3c)

$$\frac{\bar{\omega}}{\omega} = \frac{\alpha K}{\beta} + \frac{\hat{\omega}}{\hat{\omega}}$$  \hfill (4.4a)

$$\frac{\bar{\bar{\omega}}}{\omega} = \frac{K}{q\lambda} + \frac{\hat{\omega}}{q\lambda^2 \hat{\omega}}$$  \hfill (4.4b)

$$\frac{\bar{\bar{\bar{\omega}}}}{\omega} = \frac{K \lambda}{\beta} + \frac{\hat{\omega}}{\alpha \hat{\omega}}$$  \hfill (4.4c)

The expression relating $\circ$, $\bar{\circ}$ and $\hat{\circ}$ directions is given by transforming equation (3.11) to $\omega$ variables

$$\bar{\omega} = \frac{\lambda \left( (-\alpha^2 + \beta^2) \bar{\omega} - \gamma \omega (\alpha \bar{\omega} - \beta \lambda \bar{\omega}) \right) K}{\beta \left( -1 + q\lambda^2 \right) \left( \beta \bar{\omega} - \alpha \hat{\omega} \right)}.$$  \hfill (4.5)
Using the fact $\omega = \tilde{\omega}$, we see that the inner 3-cube in figure 4 collapses to a hexagon, and similarly for the outer 3-cube using $\tilde{\tilde{\omega}}$. Iterations of these provide two copies of the triangular lattice drawn in figure 5.

Every vertex on the lower triangular lattice in figure 5 can be calculated from the four initial conditions $\omega, \tilde{\omega}, \hat{\omega}, \tilde{\hat{\omega}}$, using the three quad-equations (4.3a)–(4.3c). (Vertices $\hat{\omega}, \tilde{\hat{\omega}}$ are calculated using (4.3a), (4.3b) and (4.3c) respectively.) Equation (4.5) provides a link between the upper and lower triangular lattices. In this way, we find that the iteration in the $\circ$ direction (or $k$ direction) provides layers of triangular lattices. See figure 5.

Without the $(1, 1, 1)$-periodic condition, the $H^3$ system cannot be embedded into the layered triangular lattice which has affine Weyl symmetry $\tilde{W}(A_2 + A_1)^{(1)}$, which we call here $\tilde{A}_1^{(1)}$ lattice. So the system provided above is a reduction of the $H^3$ system on a 4-cube. To show that the reduced 4-cube system is indeed $q$-Painlevé system on $A_1^{(1)}$-surface, we define

$$f = \frac{\tilde{\omega}}{\omega}, \quad g = \lambda \frac{\tilde{\tilde{\omega}}}{\omega}$$

and find their shifts in the $\bar{\bar{\circ}}$ direction, i.e., $\tilde{f} = \frac{\bar{\bar{\omega}}}{\bar{\bar{\tilde{\omega}}}}, \tilde{g} = \lambda \frac{\bar{\bar{\tilde{\tilde{\omega}}}}}{\bar{\bar{\omega}}}$. For $\hat{\omega}$, we use (4.3b), shifted one step in $\bar{\bar{\circ}}$ and one step in $\bar{\bar{\circ}}$, along with the periodic condition (4.2). For $\tilde{\omega}$, we shift (4.3a) one step in $\bar{\bar{\circ}}$. These provide

$$\tilde{\tilde{\omega}} = \frac{qa\omega \tilde{\omega} + \gamma \omega \hat{\omega}}{\gamma \odot + qa\omega \hat{\omega}}, \quad \tilde{\hat{\omega}} = \frac{\beta \lambda \odot \tilde{\tilde{\omega}} + q\alpha \lambda^2 \tilde{\hat{\omega}}}{qa\odot + \beta \lambda \odot \hat{\omega}}.$$  

Thus we have

$$\tilde{g} = \frac{\lambda^2(1 + ft)}{fg(f + t)}, \quad \tilde{f} = \frac{\lambda^2(1 + agt)}{fg(\tilde{g} + at)},$$

where we have let

$$t = qa/\gamma, \quad a = \gamma / \beta$$

and $t$ is the independent variable of the $q$-Painlevé equation and $a$ is a parameter. The system (4.8) is the third $q$-discrete Painlevé equation ($q$-$P_{III}$) [23].

The triangular lattices in figure 5 also provide a direct way of constructing the Bäcklund transformations of system (4.8). For translation in the $\circ$ direction for $g$ and $f$ we have

$$\tilde{\bar{\bar{g}}} = q\bar{\bar{\omega}}/\bar{\bar{\odot}} \quad \text{and} \quad \tilde{\bar{\bar{f}}} = \bar{\bar{\tilde{\omega}}}/\bar{\bar{\odot}}.$$

For $\hat{\omega}$ we use the equation on the face containing $\tilde{\omega}, \hat{\omega}, \tilde{\tilde{\omega}}, \hat{\tilde{\omega}}$ and the periodic condition (4.2). These lead to

$$\tilde{\odot} = \omega \left( \frac{K\bar{\bar{\odot}}}{\gamma \beta} \right)$$

Using (4.5), (4.10), and (4.4a) we have

$$\tilde{\bar{\bar{g}}} = \frac{q(fgq + a ft + a)}{g(fgq + a ft + aq\lambda^2)}, \quad \tilde{\bar{\bar{f}}} = \frac{q(fgq + a ft + a\lambda^2)}{f(fgq + a ft + a)},$$

which describe the Bäcklund transformation of $f$ and $g$, also known as the fourth $q$-discrete Painlevé equation ($q$-$P_{IV}$).
4.1. (2, 1) Staircase reduction.

We now explain how different types of staircases taken on a 2D square lattice are actually sub-cases of the geometric reduction on the $n$-cube. We demonstrate this by investigating the only sub-case of the reduction considered in the previous section.

Let $l = n, \alpha = \gamma, \ (\text{i.e., } \sim)$ then the $(1, 1, 1)$-periodicity $\tilde{\omega} = \omega$ becomes the $(2, 1)$-periodicity $\tilde{\omega} = \omega$. (4.12)

System (4.3a)-(4.4c) reduces to one equation, i.e. equation (4.3a) with the condition $\tilde{a} / \alpha = \tilde{b} / \beta = q^2$. Using the same definition (4.6) for $f$ and $g$, and (4.9) for $t$ and $a$, we find

\[ \tilde{g} = \frac{\lambda^2}{g'f'}, \quad \tilde{f} = \frac{g(atg + 1)}{\lambda(g + at)}, \]  

which can be rewritten as a single equation for $g$

\[ \tilde{g} = \frac{\lambda^3(g + at)}{gg(atg + 1)}. \]  

The resulting equation is the symmetric version of $q$-P$_{III}$ (4.8), usually referred to as $q$-P$_{II}$. This correspondence between $(1, 1, 1)$ and $(2, 1)$ reductions can be explained by projective reduction from the viewpoint of $\omega$-lattice [14].

5. Conclusion

In this paper, we provided a new method called ‘geometric reduction’ that relates ABS equations to discrete Painlevé equations. The method relies on the identification of an $n$-cube with the Voronoi cell of the root lattice of $\mathcal{W}(A_{n-1})$. As an example, we constructed a $q$-Painlevé equation from an asymmetric system based on the $H^3$ and $H^6$ type equations on a 4-cube and provided the reduction to its symmetric form as its 2D sub-case. We also answered here a question posed at the end of [22] whether a gauge transformation (4.1) can be explained by the symmetry. It turns out to be the $\mathcal{W}(A_1^{(1)})$ part of the full symmetry of the Painlevé system associated with rational surface of type $A_5^{(1)}$, i.e., its Bäcklund transformation. Bäcklund transformations of the discrete Painlevé equation arise as a natural by-product of our construction. Obtaining other structures related to integrability, such as Lax pairs, is also possible and will be reported in a separate paper. An interesting future direction is to extend our method to other types of discrete Painlevé equations classified by Sakai [23], and moreover to understand its relations with other types of higher dimensional integrable systems [15, 24, 25].

Acknowledgments

The authors would like to express their sincere thanks to Drs J Atkinson, P Kassotakis and P McNamara for inspiring and fruitful discussions.
Appendix. The generators of $\widetilde{\mathcal{W}}((A_2 + A_1)^{(1)})$ and the triangular lattice

The affine Weyl group $\widetilde{\mathcal{W}}((A_2 + A_1)^{(1)})$ is generated by $s_0, s_1, s_2, \pi, w_0, w_1, r$, which are transformations of parameters and variables that satisfy the fundamental relations

$$s_0^2 = (s_i s_{i+1})^3 = \pi^3 = 1, \quad \pi s_i = s_{i+1} \pi, \quad (i \in \mathbb{Z}/3\mathbb{Z}), \quad (A.1)$$

$$w_0^2 = w_1^2 = r^2 = 1, \quad r w_0 = w_1 r. \quad (A.2)$$

Here, the action of $\tilde{\mathcal{W}}(A_2^{(1)}) = \langle s_0, s_1, s_2, \pi \rangle$ and that of $\tilde{\mathcal{W}}(A_1^{(1)}) = \langle w_0, w_1, r \rangle$ commute. Full details of how to construct this affine Weyl group from the $\omega$-lattice can be found in [14], with the identification $\omega = \omega_0$. Here we point out how this construction can be related to the triangular lattice shown in figure 5.

Define the translations $T_i$ ($i = 1, 2, 3, 4$) by

$$T_1 = \pi s_2 s_1, \quad T_2 = \pi s_0 s_2, \quad T_3 = \pi s_1 s_0, \quad T_4 = r w_0, \quad (A.3)$$

where $T_i$ ($i = 1, 2, 3$) are translations of $\tilde{\mathcal{W}}(A_2^{(1)})$ and $T_4$ is a translation of $\tilde{\mathcal{W}}(A_1^{(1)})$.

We connect these generators to the triangular lattice in figure 5 by identifying

$$T_1: (a_0, a_1, a_2, \lambda) \mapsto (qa_0, qa_1, a_2, \lambda) \Leftrightarrow: l \mapsto l + 1,$$

$$T_2: (a_0, a_1, a_2, \lambda) \mapsto (a_0, qa_1, q^{-1}a_2, \lambda) \Leftrightarrow: m \mapsto m + 1,$$

$$T_3: (a_0, a_1, a_2, \lambda) \mapsto (q^{-1}a_0, a_1, qa_2, \lambda) \Leftrightarrow: n \mapsto n + 1,$$

$$T_2: (a_0, a_1, a_2, \lambda) \mapsto (a_0, a_1, a_2, qa_0) \Leftrightarrow: k \mapsto k + 1.$$

The periodicity condition $\delta = \omega$ corresponds to the relation $T_1 T_2 T_3 = 1$ of $\tilde{\mathcal{W}}(A_2^{(1)})$.

References

[1] Adler V E, Bobenko A and Suris Y B 2003 Classification of integrable equations on quad-graphs. The consistency approach Commun. Math. Phys. 233 513–43
[2] Adler V E, Bobenko A I and Suris Y B 2009 Discrete nonlinear hyperbolic equations. Classification of integrable cases. Funct. Anal. Appl. 43 3–17
[3] Atkinson J 2008 Bäcklund transformations for integrable lattice equations J. Phys. A: Math. Theor. 41 135202
[4] Boll R 2011 Classification of 3D consistent quad-equations J. Nonlinear Math. Phys. 18 337–65
[5] Boll R 2012 Corrigendum: ‘classification of 3D consistent quad-equations’ J. Nonlinear Math. Phys. 19 1292001–1–1292001–3
[6] Boll R 2013 On Bianchi permutability of Bäcklund transformations for asymmetric quad-equations J. Nonlinear Math. Phys. 20 577–605
[7] Conway J H and Sloane N J A 1999 Sphere Packings, Lattices and Groups (Grundlehren der Mathematischen Wissenschaften[Fundamental Principles of Mathematical Sciences] vol 290) 3rd edn (New York: Springer) With additional contributions by E Bannai, R E Borcherds, J Leech, S P Norton, A M Odlyzko,R A Parker, L Queen and B B Venkov.
[8] Field C M, Joshi N and Nijhoff F W 2008 q-difference equations of KdV type and Chazy-type second-degree difference equations J. Phys. A: Math. Theor. 41 332005
[9] Grammaticos B, Ramani A, Satsuma J, Willox R and Carstea A 2005 Reductions of integrable lattices J. Nonlinear Math. Phys. 12 363–71
[10] Hay M, Hietarinta J, Joshi N and Nijhoff F 2006 A Lax pair for a lattice modified KdV equation, reductions to q-Painlevé equations and associated Lax pairs J. Phys. A: Math. Theor. 40 F61
[11] Hay M, Howes P and Shi. Y 2013 A systematic approach to reductions of type-Q ABS equations arXiv:1307.3390
[12] Humphreys J E 1990 Reflection Groups and Coxeter Groups (Cambridge Studies in Advanced Mathematics vol 29) (Cambridge: Cambridge University Press)
13 Joshi N, Grammaticos B, Tamizhmani T and Ramani A 2006 From integrable lattices to non-QRT mappings Lett. Math. Phys. 78 27–37
14 Joshi N, Nakazono N and Shi Y 2014 ABS equations arising from discrete Painlevé systems (I): \((A_2 + A_1)^{(1)}\) and \((A_3 + A_1)^{(1)}\) cases arXiv:1401.7044
15 Kajiwara K, Noumi M and Yamada Y 2002 q-Painlevé systems arising from q-KP hierarchy Lett. Math. Phys. 62 259–68
16 Moody R V and Patera J 1992 Voronoï and Delaunay cells of root lattices: classification of their faces and facets by Coxeter–Dynkin diagrams J. Phys. A: Math. Gen. 25 5089–134
17 Nijhoff F and Papageorgiou V 1991 Similarity reductions of integrable lattices and discrete analogues of the Painlevé II equation Phys. Lett. A 153 337–44
18 Nijhoff F W and Walker A J 2001 The discrete and continuous Painlevé VI hierarchy and the Garnier systems Glass. Math. J. 43A 109–23
19 Noumi M 2004 Painlevé Equations Through Symmetry (Translations of Mathematical Monographs vol 223) (Providence, RI: American Mathematical Society) Translated from the 2000 Japanese original by the author
20 Okamoto K 1979 Sur les feuilletages associés aux équations du second ordre à points critiques fixes de P. Painlevé, espaces des conditions initiales Science Council of Japan Jap. J. Math. New Ser. 5 1–79
21 Ormerod C M 2012 Reductions of lattice mKdV to q-R\(_{1,1}\) Phys. Lett. A 376 2855–9
22 Ormerod C M 2014 Symmetries and special solutions of reductions of the lattice potential KdV equation Symmetry Integrability Geom. Methods Appl. 10 02–19
23 Sakai H 2001 Rational surfaces associated with affine root systems and geometry of the Painlevé equations Commun. Math. Phys. 220 165–229
24 Tsuda T 2009 Universal character and q-difference Painlevé equations Math. Ann. 345 395–415
25 Tsuda T 2010 On an integrable system of q-difference equations satisfied by the universal characters: its Lax formalism and an application to q-Painlevé equations Commun. Math. Phys. 293 347–59
26 Tsuda T 2012 From KP/UC hierarchies to Painlevé equations Int. J. Math. 23 1250010 59
27 Willox R and Hietarinta J 2006 On the bilinear forms of Painlevé’s 4th equation, Bilinear Integrable Systems: From Classical to Quantum, Continuous to Discrete (NATO Science Series II Mathematics Physics Chemistry vol 201) (Dordrecht: Springer) pp 375–90