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Integrable Boundary Interactions for Ruijsenaars' Difference Toda Chain

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Abstract: We endow Ruijsenaars' open difference Toda chain with a one-sided boundary interaction of Askey–Wilson type and diagonalize the quantum Hamiltonian by means of deformed hyperoctahedral q-Whittaker functions that arise as a $t = 0$ degeneration of the Macdonald–Koornwinder multivariate Askey–Wilson polynomials. This immediately entails the quantum integrability, the bispectral dual system, and the n-particle scattering operator for the chain in question.

1. Introduction

It is well-known that the open and closed Toda chains may be viewed as limits of the hyperbolic and elliptic Calogero–Moser–Sutherland particle systems, respectively [St,R1,I,R2]. More general integrable open Toda chains with boundary interactions involving potentials of Morse type [Ko,GW,Sk1] and of Pöschl-Teller type [I,KJC] are recovered similarly as degenerations of the Olshanetsky–Perelomov–Inozemtsev generalized Calogero–Moser–Sutherland systems with hyperoctahedral symmetry [I,O,Sh,GLO2]. Moreover, such limiting relations turn out to persist at the level of the Ruijsenaars-Schneider particle systems and Ruijsenaars' difference (a.k.a. relativistic) Toda chains [R1,R2,R3,E,GLO1,HR,BC], as well as their hyperoctahedral counterparts [D2,C]. Specifically, in the hyperoctahedral case one recovers in this manner generalizations of Ruijsenaars' open relativistic Toda chain with boundary interactions that were studied at the level of classical mechanics in Refs. [Su1,D1,Su2] and at the level of quantum mechanics in Refs. [KT,D2,E,S,C].

In the present work we consider the Hamiltonian of such an open difference Toda chain endowed with a one-sided four-parameter boundary interaction of Askey–Wilson type. Upon diagonalizing the quantum Hamiltonian in question by means of deformed

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hyperoctahedral q-Whittaker functions that arise as a $t = 0$ degeneration of the Macdonald–Koornwinder polynomials [K,M], the quantum integrability, the bispectral dual system, and the n-particle scattering operator are deduced. For special values of the Askey–Wilson parameters, our chain amounts to a difference counterpart of the D_n-type and the A_{n-1}-type quantum Toda chains with one-sided boundary potentials of Pöschl-Teller and Morse type, respectively.

The presentation is structured as follows. After introducing our difference Toda chain in Sect. 2 and defining the deformed hyperoctahedral q-Whittaker functions in Sect. 3, the diagonalization of the Hamiltonian is carried out in Sect. 4 by identifying the corresponding eigenvalue equation with the $t \to 0$ degeneration of a well-known Pieri formula for the Macdonald–Koornwinder polynomials [D3,M]. The quantum integrals and the bispectral dual system are then discussed in Sects. 5 and 6, respectively. In Sect. 7 analogous results for a difference counterpart of the quantum Toda chain with one-sided boundary potentials of Morse type are obtained by letting one of the boundary parameters tend to zero (which corresponds to a transition from Askey–Wilson polynomials to continuous dual q-Hahn polynomials [KLS]). We close in Sect. 8 with an explicit description of the n-particle scattering operator that relies on a stationary-phase analysis that was performed in Refs. [R4,D4]. Some useful properties of the Macdonald–Koornwinder multivariate Askey–Wilson polynomials have been collected in a separate appendix at the end.

2. Difference Toda Chain with One-Sided Boundary Interaction of Askey–Wilson Type

Formally, the Hamiltonian of our difference Toda chain is given by the difference operator [D2]:

$$\begin{aligned} H := T_1 &+ \sum_{j=2}^{n-1}(1-q^{x_{j-1}-x_j})T_j \\ &+ \sum_{j=1}^{n-2}(1-q^{x_j-x_{j+1}})T_j^{-1} + (1-q^{x_{n-1}-x_n})(1-q^{x_{n-1}+x_n})T_{n-1}^{-1} \\ &+ w_+(x_n)(1-q^{x_{n-1}-x_n})T_n + w_-(x_n)(1-q^{x_{n-1}+x_n})T_n^{-1} + U(x_{n-1},x_n), \end{aligned} \tag{2.1a}$$

where

$$w_+(x) := \frac{\prod_{0\le r\le 3}(1-t_rq^x)}{(1-q^{2x})(1-q^{2x+1})}, \quad w_-(x) := \frac{\prod_{0\le r\le 3}(1-t_r^{-1}q^x)}{(1-q^{2x})(1-q^{2x-1})}, \tag{2.1b}$$

$$U(x,y) := \sum_{\epsilon\in\{1,-1\}} \frac{c_\epsilon(1-\epsilon q^{x+1/2})}{(1-\epsilon q^{y-1/2})(1-\epsilon q^{-y-1/2})}, \tag{2.1c}$$

with

$$c_\epsilon := \frac{1}{2\sqrt{q^{-1}t_0t_1t_2t_3}} \prod_{0\le r\le 3}(1-\epsilon q^{-1/2}t_r), \tag{2.1d}$$

and T_j $(j = 1,\ldots,n)$ acts on functions $f : \mathbb{R}^n \to \mathbb{C}$ by a unit translation of the jth position variable

$$(T_jf)(x_1,\ldots,x_n) = f(x_1,\ldots,x_{j-1},x_j+1,x_{j+1},\ldots,x_n).$$

Here q denotes a scale parameter and the parameters t_r ($r = 0, \ldots, 3$) play the role of coupling parameters for the boundary interaction of Askey–Wilson type. Upon setting $t_2 = -t_3 = q^{1/2}$, the additive potential term $U(x_{n-1}, x_n)$ in H (2.1a)–(2.1d) vanishes. The above Toda chain amounts in this case to a difference analog of the previously studied D_n-type quantum Toda chain with Pöschl-Teller boundary potential [I,KJC,O,GLO2]. If we additionally set $t_0 = -t_1 = 1$, then $w_+(x) = w_-(x) = 1$ and we formally recover a D_n-type analog of Ruijsenaars' difference Toda chain [KT,E,S,C] that was introduced at the level of classical mechanics by Suris [Su1].

3. Deformed Hyperoctahedral q-Whittaker Functions

Let Λ denote the cone of integer partitions $\lambda = (\lambda_1, \ldots, \lambda_n)$ with decreasingly ordered parts $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$, and let W be the hyperoctahedral group formed by the semi-direct product of the symmetric group S_n and the n-fold product of the cyclic group $\mathbb{Z}_2 \cong \{1, -1\}$. Elements $w = (\sigma, \epsilon) \in W$ act naturally on $\xi = (\xi_1, \ldots \xi_n) \in \mathbb{R}^n$ via $w\xi := (\epsilon_1 \xi_{\sigma_1}, \ldots, \epsilon_n \xi_{\sigma_n})$ (with $\sigma \in S_n$ and $\epsilon_j \in \{1, -1\}$ for $j = 1, \ldots, n$). A standard basis for the algebra of W-invariant trigonometric polynomials on the torus $\mathbb{T} = \mathbb{R}^n/(2\pi\mathbb{Z}^n)$ is given by the hyperoctahedral monomial symmetric functions

$$m_\lambda(\xi) := \sum_{\mu \in W\lambda} e^{i\langle \mu, \xi \rangle}, \qquad \lambda \in \Lambda, \tag{3.1}$$

where the summation is meant over the orbit of λ with respect to the action of W and the bracket $\langle \cdot, \cdot \rangle$ refers to the usual inner product on $\mathbb{R}^n$ (so $\langle \mu, \xi \rangle = \mu_1 \xi_1 + \cdots + \mu_n \xi_n$). This monomial basis inherits a natural partial order from the hyperoctahedral dominance ordering of the partitions:

$$\forall \mu, \lambda \in \Lambda: \quad \mu \leq \lambda \text{ iff } \sum_{1 \leq j \leq k} \mu_j \leq \sum_{1 \leq j \leq k} \lambda_j \quad \text{for} \quad k = 1, \ldots, n. \tag{3.2}$$

By definition, the basis of deformed hyperoctahedral q-Whittaker functions $p_\lambda(\xi)$, $\lambda \in \Lambda$ is given by the polynomials of the form

$$p_\lambda(\xi) = m_\lambda(\xi) + \sum_{\substack{\mu \in \Lambda \\ \text{with } \mu < \lambda}} c_{\lambda,\mu} m_\mu(\xi) \qquad (c_{\lambda,\mu} \in \mathbb{C}) \tag{3.3a}$$

such that

$$\langle p_\lambda, m_\mu \rangle_{\hat{\Delta}} = 0 \quad \text{if } \mu < \lambda, \tag{3.3b}$$

where the inner product

$$\langle \hat{f}, \hat{g} \rangle_{\hat{\Delta}} := \int_{\mathbb{A}} \hat{f}(\xi) \overline{\hat{g}(\xi)} \hat{\Delta}(\xi) \mathrm{d}\xi \qquad (\hat{f}, \hat{g} \in L^2(\mathbb{A}, \hat{\Delta}(\xi)\mathrm{d}\xi)) \tag{3.4a}$$

is determined by the weight function

$$\hat{\Delta}(\xi) := \frac{1}{(2\pi)^n} \prod_{1 \leq j < k \leq n} \left| (e^{i(\xi_j + \xi_k)}, e^{i(\xi_j - \xi_k)})_\infty \right|^2 \prod_{1 \leq j \leq n} \left| \frac{(e^{2i\xi_j})_\infty}{\prod_{0 \leq r \leq 3} (\hat{t}_r e^{i\xi_j})_\infty} \right|^2 \tag{3.4b}$$

supported on the hyperoctahedral Weyl alcove

$$\mathbb{A} := \{(\xi_1, \xi_2, \ldots, \xi_n) \in \mathbb{R}^n \mid \pi > \xi_1 > \xi_2 > \cdots > \xi_n > 0\}. \quad (3.5)$$

Here $(x)_m := \prod_{l=0}^{m-1}(1 - xq^l)$ and $(x_1, \ldots, x_l)_m := (x_1)_m \cdots (x_l)_m$ refer to standard notations for the q-Pochhammer symbols, and it is assumed that

$$q \in (0, 1) \quad \text{and} \quad \hat{t}_r \in (-1, 1)\setminus\{0\} \quad (r = 0, \ldots, 3). \quad (3.6)$$

These deformed hyperoctahedral q-Whittaker functions $p_\lambda(\xi), \lambda \in \Lambda$ amount to a $t \to 0$ degeneration of the more general Macdonald-Koorwinder multivariate Askey–Wilson polynomials introduced in Ref. [K] (cf. Appendix A below).

4. Diagonalization

It is known that the eigenfunctions of Ruijsenaars' open difference Toda chain consist of A_{n-1}-type q-Whittaker functions given by a $t \to 0$ limit of the Macdonald symmetric functions [GLO1]. In this section our aim is to show that an analogous result holds for the chain with Askey-Wilson type boundary interactions from Sect. 2, upon employing the deformed hyperoctahedral q-Whittaker functions from Sect. 3. To this end it is convenient to reparametrize the boundary parameters of the Toda chain in terms of the q-Whittaker deformation parameters (3.6) via

$$t_0 = \sqrt{q^{-1}\hat{t}_0\hat{t}_1\hat{t}_2\hat{t}_3}, \qquad t_r = \hat{t}_r\hat{t}_0/t_0 \quad (r = 1, 2, 3), \quad (4.1)$$

assuming (from now onwards) the additional positivity constraints

$$\hat{t}_0 > 0 \quad \text{and} \quad \hat{t}_0\hat{t}_1\hat{t}_2\hat{t}_3 > 0. \quad (4.2)$$

Let $\rho_0 + \Lambda := \{\rho_0 + \lambda \mid \lambda \in \Lambda\}$ with

$$\rho_0 := (\log_q(t_0), \ldots, \log_q(t_0)) \in \mathbb{R}^n.$$

We write $\ell^2(\rho_0 + \Lambda, \Delta)$ for the Hilbert space of lattice functions $f : (\rho_0 + \Lambda) \to \mathbb{C}$ determined by the inner product

$$\langle f, g\rangle_\Delta := \sum_{\lambda\in\Lambda} f(\rho_0 + \lambda)\overline{g(\rho_0 + \lambda)}\Delta_\lambda \qquad (f, g \in \ell^2(\rho_0 + \lambda_n, \Delta)), \quad (4.3a)$$

where

$$\Delta_\lambda := \frac{\Delta_0}{(qt_0^2)_{\lambda_{n-1}+\lambda_n}}\left(\frac{1 - t_0^2q^{2\lambda_n}}{1 - t_0^2}\right)\prod_{0\le r\le 3}\frac{(t_0t_r)_{\lambda_n}}{(qt_0t_r^{-1})_{\lambda_n}}\prod_{1\le j<n}\frac{1}{(q)_{\lambda_j-\lambda_{j+1}}} \quad (4.3b)$$

and

$$\Delta_0 := (q)_\infty \prod_{0\le r<s\le 3}\left(\hat{t}_r\hat{t}_s\right)_\infty = (q)_\infty \prod_{1\le r\le 3}(t_0t_r, qt_0t_r^{-1})_\infty. \quad (4.3c)$$

From the limiting behavior for $t \to 0$ of the orthogonality relations satisfied by the normalized Macdonald–Koornwinder polynomials (A.2a)–(A.2c), it is immediate that the wave function

$$\psi_\xi(\rho_0 + \lambda) := \frac{(t_0^2)_{2\lambda_n}}{\prod_{0\le r\le 3}(t_0t_r)_{\lambda_n}}p_\lambda(\xi) \qquad (\lambda \in \Lambda,\ \xi \in \mathbb{A}) \quad (4.4)$$

satisfies the following orthogonality with respect to the spectral variable ξ:

$$\int_{\mathbb{A}} \psi(\rho_0+\lambda)\overline{\psi(\rho_0+\mu)}\hat{\Delta}(\xi)\mathrm{d}\xi = \begin{cases} \Delta_\lambda^{-1} & \text{if } \lambda=\mu, \\ 0 & \text{otherwise.} \end{cases} \tag{4.5}$$

In other words, the corresponding Fourier transform $\boldsymbol{F} : \ell^2(\rho_0+\Lambda, \Delta) \to L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$ given by

$$(\boldsymbol{F} f)(\xi) := \langle f, \psi_\xi\rangle_\Delta = \sum_{\lambda\in\Lambda} f(\rho_0+\lambda)\overline{\psi_\xi(\rho_0+\lambda)}\Delta_\lambda \tag{4.6a}$$

($f \in \ell^2(\rho_0+\Lambda, \Delta)$) constitutes a Hilbert space isomorphism with an inversion formula of the form

$$(\boldsymbol{F}^{-1}\hat{f})(\rho_0+\lambda) = \langle \hat{f}, \overline{\psi(\rho_0+\lambda)}\rangle_{\hat{\Delta}} = \int_{\mathbb{A}} \hat{f}(\xi)\psi_\xi(\rho_0+\lambda)\hat{\Delta}(\xi)\mathrm{d}\xi \tag{4.6b}$$

($\hat{f} \in L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$). We will refer to $\boldsymbol{F}$ (4.6a), (4.6b) as the deformed hyperoctahedral q-Whittaker transform.

The formal Hamiltonian H (2.1a)–(2.1d) restricts to a well-defined discrete difference operator in the space of complex functions on the lattice $\rho_0+\Lambda$. Indeed, when $t_0 \notin \{1, q^{1/2}\}$ it is manifest that for $x=(x_1,\ldots,x_n)$ at these lattice points we stay away from the poles in the coefficients of H stemming from the denominators of $w_\pm(x_n)$ and $U(x_{n-1},x_n)$ and, moreover, that for any $f:\mathbb{R}^n\to\mathbb{C}$ and any $\lambda\in\Lambda$ the value of $(Hf)(\rho_0+\lambda)$ depends only on evaluations of f at points of $\rho_0+\Lambda$ (due to the vanishing of $(1-q^{\lambda_j-\lambda_{j+1}})$ at $\lambda_j=\lambda_{j+1}$ ($1\le j<n$) and the vanishing of $w_-(\log_q(t_0)+\lambda_n)$ at $\lambda_n=0$):

$$\begin{aligned}(Hf)(\rho_0+\lambda) \\ = \sum_{\substack{1\le j\le n\\ \lambda+e_j\in\Lambda}} v_j^+(\lambda) f(\rho_0+\lambda+e_j) + \sum_{\substack{1\le j\le n\\ \lambda-e_j\in\Lambda}} v_j^-(\lambda) f(\rho_0+\lambda-e_j) + u(\lambda) f(\rho_0+\lambda),\end{aligned} \tag{4.7}$$

where

$$\begin{aligned}
v_j^+(\lambda) &= (1-q^{\lambda_{j-1}-\lambda_j})\left(\frac{\prod_{0\le r\le 3}(1-t_r t_0 q^{\lambda_n})}{(1-t_0^2q^{2\lambda_n})(1-t_0^2q^{2\lambda_n+1})}\right)^{\delta_{n-j}}, \\
v_j^-(\lambda) &= (1-q^{\lambda_j-\lambda_{j+1}})(1-t_0^2q^{\lambda_{n-1}+\lambda_n})^{\delta_{n-j}+\delta_{n-1-j}} \\
&\quad\times\left(\frac{\prod_{0\le r\le 3}(1-t_r^{-1}t_0q^{\lambda_n})}{(1-t_0^2q^{2\lambda_n})(1-t_0^2q^{2\lambda_n-1})}\right)^{\delta_{n-j}}, \\
u(\lambda) &= \sum_{\epsilon\in\{1,-1\}} \frac{c_\epsilon(1-\epsilon t_0q^{\lambda_{n-1}+1/2})}{(1-\epsilon t_0 q^{\lambda_n-1/2})(1-\epsilon t_0^{-1}q^{-\lambda_n-1/2})},
\end{aligned}$$

with c_ϵ taken from (2.1d). Here $\delta_k := 1$ if $k=0$ and $\delta_k := 0$ otherwise, the vectors $e_1,\ldots,e_n$ denote the standard unit basis of $\mathbb{R}^n$, and $\lambda_0 := +\infty$, $\lambda_{n+1} := -\infty$ by convention (so $(1-q^{\lambda_0-\lambda_1}) = (1-q^{\lambda_n-\lambda_{n+1}}) \equiv 1$). The action of H on lattice functions in Eq. (4.7) extends continuously from $t_0 \notin \{1, q^{1/2}\}$ to the full parameter domain determined by Eqs. (4.1), (4.2) and (3.6).

Our main result implements the Hamiltonian under consideration as a self-adjoint operator in the Hilbert space $\ell^2(\rho_0+\Lambda, \Delta)$ and provides its spectral decomposition with the aid of the deformed hyperoctahedral q-Whittaker transform.

Theorem 1 (Diagonalization). *(i). For boundary parameters t_r (4.1) determined by the q-Whittaker deformation parameters $\hat{t}_r$ (3.6), (4.2), the action of the difference Toda Hamiltonian H (2.1a)–(2.1d) given by Eq. (4.7) constitutes a bounded self-adjoint operator in the Hilbert space $\ell^2(\rho_0+\Lambda, \Delta)$ with purely absolutely continuous spectrum. (ii). The operator in question is diagonalized by the deformed hyperoctahedral q-Whittaker transform $\boldsymbol{F}$ (4.6a), (4.6b):*

$$H = \boldsymbol{F}^{-1} \circ \hat{E} \circ \boldsymbol{F}, \tag{4.8a}$$

where $\hat{E}$ denotes the bounded real multiplication operator acting on $\hat{f} \in L^2(\mathbb{A}, \hat{\Delta} d\xi)$ via

$$(\hat{E}\hat{f})(\xi) := \hat{E}(\xi)\hat{f}(\xi) \quad \textit{with} \quad \hat{E}(\xi) := 2 \sum_{1\le j\le n} \cos(\xi_j). \tag{4.8b}$$

Proof. The first part of the theorem is immediate from the second part. To prove the second part it suffices to verify that the deformed hyperoctahedral q-Whittaker kernel ψ_ξ satisfies the eigenvalue equation $H\psi_\xi = \hat{E}(\xi)\psi_\xi$, or more explicitly that:

$$\sum_{\substack{1\le j\le n\\ \lambda+e_j\in\Lambda}} v_j^+(\lambda)\psi_\xi(\rho_0+\lambda+e_j) + \sum_{\substack{1\le j\le n\\ \lambda-e_j\in\Lambda}} v_j^-(\lambda)\psi_\xi(\rho_0+\lambda-e_j)$$
$$+u(\lambda)\psi_\xi(\rho_0+\lambda) = \hat{E}(\xi)\psi_\xi(\rho_0+\lambda).$$

This eigenvalue equation follows from the Pieri formula for the Macdonald–Koornwinder polynomials (A.4) in the limit $t \to 0$. Indeed, it is clear that in the Pieri formula $\lim_{t\to 0} \mathbf{P}_\lambda(\xi) = \psi_\lambda(\rho_0+\lambda)$, $\lim_{t\to 0} \hat{\tau}_j V_j^+(\lambda) = v_j^+(\lambda)$, $\lim_{t\to 0} \hat{\tau}_j^{-1} V_j^-(\lambda) = v_j^-(\lambda)$, and one also has that

$$\lim_{t\to 0}\left(\sum_{j=1}^n(\hat{\tau}_j+\hat{\tau}_j^{-1}) - \sum_{\substack{1\le j\le n\\ \lambda+e_j\in\Lambda}} V_j^+(\lambda) - \sum_{\substack{1\le j\le n\\ \lambda-e_j\in\Lambda}} V_j^-(\lambda)\right) = u(\lambda).$$

This last limit formula is not evident but can be deduced from the following rational identity in $q^{x_1}, \ldots, q^{x_n}$:

$$\sum_{j=1}^n\left(\hat{\tau}_j^{-1} - \hat{\tau}_1^{-1} w_+(x_j) \prod_{\substack{1\le k\le n\\ k\ne j}} \frac{1-tq^{x_j+x_k}}{1-q^{x_j+x_k}} \frac{1-tq^{x_j-x_k}}{1-q^{x_j-x_k}}\right)$$
$$+\sum_{j=1}^n\left(\hat{\tau}_j - \hat{\tau}_1 w_-(x_j) \prod_{\substack{1\le k\le n\\ k\ne j}} \frac{1-t^{-1}q^{x_j+x_k}}{1-q^{x_j+x_k}} \frac{1-t^{-1}q^{x_j-x_k}}{1-q^{x_j-x_k}}\right)$$
$$= C_t \sum_{\epsilon\in\{1,-1\}} \prod_{0\le r\le 3} (1-\epsilon t_r q^{-1/2}) \left(1 - \prod_{j=1}^n \frac{1-\epsilon t q^{x_j-1/2}}{1-\epsilon q^{x_j-1/2}} \frac{1-\epsilon t^{-1} q^{x_j+1/2}}{1-\epsilon q^{x_j+1/2}}\right),$$

where $C_t = -\frac{1}{2}t\hat{t}_0^{-1}(1-t)^{-1}(1-q^{-1}t)^{-1}$, upon replacing q^{x_j} by $\tau_j q^{\lambda_j}$ $(j = 1, \ldots, n)$ and performing the limit $t \to 0$. To infer the rational identity itself, one exploits the hyperoctahedral symmetry in the variables $x_1, \ldots x_n$ and checks that—as a function of x_j (with the remaining variables fixed in a generic configuration)—the residues at the (simple) poles on both sides coincide. Hence, the difference of both rational expressions amounts to a W-invariant Laurent polynomial in $q^{x_1}, \ldots, q^{x_n}$. The Laurent polynomial in question must actually vanish, as the rational expressions under consideration tend to 0 for $x_j = (n+1-j)c$ in the limit $c \to +\infty$. □

5. Integrability

The quantum integrability of the difference Toda Hamiltonian H (2.1a)–(2.1d) is an immediate consequence of the diagonalization in Theorem 1. In effect, a complete system of commuting quantum integrals in the Hilbert space $\ell^2(\rho_0 + \Lambda, \Delta)$ is given by the bounded self-adjoint operators

$$H_l := \boldsymbol{F}^{-1} \circ \hat{E}_l \circ \boldsymbol{F}, \qquad l = 1, \ldots, n, \tag{5.1}$$

where $\hat{E}_l : L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi) \to L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$ denotes the real multiplication operator by $\hat{E}_l(\xi) := m_{\omega_l}(\xi)$ with $\omega_l := e_1 + \cdots + e_l$ (so $H_1 = H$). The operator H_l (5.1) acts on $f \in \ell^2(\rho_0 + \Lambda, \Delta)$ as a difference operator of the form

$$(H_l f)(\rho_0 + \lambda) = \sum_{\substack{J \subset \{1,\ldots,n\}, 0 \le |J| \le l \\ \epsilon_j \in \{1,-1\}, j \in J; \lambda + e_{\epsilon J} \in \Lambda}} C_{\epsilon J}^{(l)}(\lambda) f(\rho_0 + \lambda + e_{\epsilon J}), \tag{5.2a}$$

where $e_{\epsilon J} := \sum_{j \in J} \epsilon_j e_j$, $|J|$ denotes the cardinality of $J \subset \{1, \ldots, n\}$, and the coefficients

$$C_{\epsilon J}^{(l)}(\lambda) = \lim_{t \to 0} C_{\epsilon J, t}^{(l)}(\lambda) \tag{5.2b}$$

arise as $t \to 0$ limits of the expansion coefficients in the corresponding Pieri formula for the normalized Macdonald–Koornwinder polynomials $\mathbf{P}_\lambda(\xi)$ (A.1a), (A.1b) (cf. [D3, Sec. 6]):

$$\hat{E}_l(\xi)\mathbf{P}_\lambda(\xi) = \sum_{\substack{J \subset \{1,\ldots,n\}, 0 \le |J| \le l \\ \epsilon_j \in \{1,-1\}, j \in J; \lambda + e_{\epsilon J} \in \Lambda}} C_{\epsilon J, t}^{(l)}(\lambda)\mathbf{P}_{\lambda + e_{\epsilon J}}(\xi). \tag{5.2c}$$

Notice in this connection that the Pieri expansion coefficients

$$C_{\epsilon J, t}^{(l)}(\lambda) = \boldsymbol{\Delta}_{\lambda + e_{\epsilon J}} \int_{\mathbb{A}} \hat{E}_l(\xi)\mathbf{P}_\lambda(\xi)\overline{\mathbf{P}_{\lambda + e_{\epsilon J}}(\xi)}\hat{\boldsymbol{\Delta}}(\xi)\mathrm{d}\xi$$

are continuous at $t = 0$, because the Macdonald–Koornwinder weight function $\hat{\boldsymbol{\Delta}}(\xi)$ and (thus) the polynomials $\mathbf{P}_\lambda(\xi)$, $\lambda \in \Lambda$ are continuous at this parameter value (cf. Appendix A).

In practice it turns out to be very tedious to compute the $t \to 0$ limiting coefficients $C_{\epsilon J}^{(l)}(\lambda)$ explicitly with the aid of the known explicit Pieri formulas for the Macdonald–Koornwinder polynomials in [D3, Sec. 6] beyond $l = 1$. For a particular second quantum integral belonging to the commutative algebra generated by $H_1, \ldots, H_n$, however, the required computation results to be surprisingly straightforward. More specifically: from the $t \to 0$ limiting behavior of the $r = n$ (top) Pieri formula for the Macdonald–Koornwinder polynomials in Theorem 6.1 of [D3], one readily deduces that the action on $f \in \ell^2(\rho_0 + \Lambda, \Delta)$ of the operator $H_Q := \boldsymbol{F}^{-1} \circ \hat{Q} \circ \boldsymbol{F}$, where $\hat{Q}$ refers to the self-adjoint multiplication operator in $L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$ by

$$\hat{Q}(\xi) := \prod_{j=1}^{n} (2\cos(\xi_j) - \hat{t}_0 - \hat{t}_0^{-1}),$$

is given explicitly by

$$(H_Q f)(\rho_0 + \lambda) = \sum_{\substack{J_+ \cup J_- \cup K_+ \cup K_- = \{1,\dots,n\} \\ |J_+|+|J_-|+|K_+|+|K_-|=n \\ \lambda + e_{J_+} - e_{J_-} \in \Lambda}} u_{K_+,K_-}(\lambda) v_{J_+,J_-}(\lambda) f(\rho_0 + \lambda + e_{J_+} - e_{J_-}), \tag{5.3}$$

with

$$\begin{aligned} v_{J_+,J_-}(\lambda) = &\prod_{\substack{j \in J_+ \\ j-1 \notin J_+}} (1 - q^{\lambda_{j-1} - \lambda_j}) \prod_{\substack{j \in J_- \\ j+1 \notin J_-}} (1 - q^{\lambda_j - \lambda_{j+1} - \delta_{J_+}(j+1)}) \\ &\times (1 - t_0^2 q^{\lambda_{n-1} + \lambda_n})^{\delta_{J_+^c}(n-1)\delta_{J_+^c}(n) - \delta_{J_+^c \cap J_-^c}(n-1)\delta_{J_+^c \cap J_-^c}(n)} \\ &\times (1 - t_0^2 q^{\lambda_{n-1} + \lambda_n - 1})^{\delta_{J_-}(n-1)\delta_{J_-}(n)} \, w_+(\lambda_n)^{\delta_{J_+}(n)} w_-(\lambda_n)^{\delta_{J_-}(n)} \end{aligned}$$

and

$$\begin{aligned} u_{K_+,K_-}(\lambda) = (-\hat{t}_0)^{|K_-| - |K_+|} &\prod_{\substack{k \in K_+ \\ k-1 \in K_-}} (1 - q^{\lambda_{k-1} - \lambda_k}) \prod_{\substack{k \in K_+ \\ k+1 \in K_-}} (1 - q^{\lambda_k - \lambda_{k+1} + 1}) \\ &\times (1 - t_0^2 q^{\lambda_{n-1} + \lambda_n + 1})^{\delta_{K_+}(n-1)\delta_{K_+}(n)} (1 - t_0^2 q^{\lambda_{n-1} + \lambda_n})^{\delta_{K_-}(n-1)\delta_{K_-}(n)} \\ &\times w_+(\lambda_n)^{\delta_{K_+}(n)} w_-(\lambda_n)^{\delta_{K_-}(n)}. \end{aligned}$$

Here $\delta_J : \{1, \dots, n\} \to \{0, 1\}$ denotes the characteristic function of $J \subset \{1, \dots, n\}$ and $J^c = \{1, \dots, n\} \backslash J$.

Corollary 1. *The difference Toda Hamiltonians H (4.7) and H_Q (5.3) are bounded, self-adjoint, commuting operators in $\ell^2(\rho_0 + \Lambda, \Delta)$ for which the deformed hyperoctahedral q-Whittaker functions ψ_ξ (4.4) constitute a complete system of (generalized) joint eigenfunctions corresponding to the eigenvalues $\hat{E}(\xi)$ and $\hat{Q}(\xi)$, respectively.*

6. Bispectral Dual System

For $t \to 0$ the Macdonald–Koornwinder q-difference equation (A.3) amounts to the following eigenvalue equation satisfied by the deformed hyperoctahedral q-Whittaker functions:

$$\hat{H} p_\lambda = (q^{-\lambda_1} - 1) p_\lambda \qquad (\lambda \in \Lambda), \tag{6.1}$$

with

$$\hat{H} = \sum_{j=1}^{n} \Big(\hat{v}_j(\xi)(\hat{T}_{j,q} - 1) + \hat{v}_j(-\xi)(\hat{T}_{j,q}^{-1} - 1) \Big), \tag{6.2a}$$

and

$$\hat{v}_j(\xi) = \frac{\prod_{0\leq r\leq 3}(1-\hat{t}_r e^{i\xi_j})}{(1-e^{2i\xi_j})(1-qe^{2i\xi_j})} \prod_{\substack{1\leq k\leq n\\ k\neq j}} (1-e^{i(\xi_j+\xi_k)})^{-1}(1-e^{i(\xi_j-\xi_k)})^{-1}, \tag{6.2b}$$

where $\hat{T}_{j,q}$ acts on trigonometric (Laurent) polynomials $\hat{p}(e^{i\xi_1},\ldots,e^{i\xi_n})$ by a q-shift of the jth variable:

$$(\hat{T}_{j,q}\hat{p})(e^{i\xi_1},\ldots,e^{i\xi_n}) := \hat{p}(e^{i\xi_1},\ldots,e^{i\xi_{j-1}},qe^{i\xi_j},e^{i\xi_{j+1}},\ldots,e^{i\xi_n}).$$

The following proposition is now immediate.

Proposition 1 (Bispectral Dual Hamiltonian). *The $t=0$ Macdonald–Koornwinder q-difference operator $\hat{H}$ (6.2a), (6.2b) constitutes a nonnegative unbounded self-adjoint operator with purely discrete spectrum in $L^2(\mathbb{A},\hat{\Delta}d\xi)$ that is diagonalized by the (inverse) deformed hyperoctahedral q-Whittaker transform $\boldsymbol{F}$ (4.6a), (4.6b):*

$$\hat{H} = \boldsymbol{F}\circ E\circ \boldsymbol{F}^{-1}, \tag{6.3a}$$

where E denotes the self-adjoint multiplication operator in $\ell^2(\rho_0+\Lambda,\Delta)$ of the form

$$(Ef)(\rho_0+\lambda) := (q^{-\lambda_1}-1)f(\rho_0+\lambda) \qquad (\lambda\in\Lambda) \tag{6.3b}$$

(for $f\in\ell^2(\rho_0+\Lambda,\Delta)$ with $\langle Ef,Ef\rangle_\Delta<\infty$).

One learns from Theorem 1 and Proposition 1 that the eigenfunction transforms diagonalizing the difference Toda Hamiltonian H (4.7) and the $t=0$ Macdonald–Koornwinder difference operator $\hat{H}$ (6.2a), (6.2b) are inverses of each other. This fact encodes the bispectral duality of the operators under consideration in the sense of Duistermaat and Grünbaum [DG, G]: the kernel function $\psi_\xi(\rho_0+\lambda)$ of the deformed hyperoctahedral q-Whittaker transform $\boldsymbol{F}$ (4.6a), (4.6b) simultaneously solves the corresponding eigenvalue equations for H and $\hat{H}$ in the discrete variable $\rho_0+\lambda$ and the spectral variable ξ, respectively.

Explicit commuting quantum integrals for the dual Hamiltonian $\hat{H}$ (6.2a), (6.2b) are obtained as a $t\to 0$ degeneration of the commuting difference operators in [D3, Thm. 5.1]:

$$\hat{H}_l = \sum_{\substack{J\subset\{1,\ldots,n\},\,0\leq|J|\leq l\\ \epsilon_j\in\{1,-1\},\,j\in J}} \hat{U}_{J^c,l-|J|}\hat{V}_{\epsilon J}\hat{T}_{\epsilon J,q}, \qquad l=1,\ldots,n, \tag{6.4}$$

with $\hat{T}_{\epsilon J,q} := \prod_{j\in J}\hat{T}_{j,q}^{\epsilon_j}$ and

$$\hat{V}_{\epsilon J} := \prod_{j\in J}\frac{\prod_{0\leq r\leq 3}(1-\hat{t}_r e^{i\epsilon_j\xi_j})}{(1-e^{2i\epsilon_j\xi_j})(1-qe^{2i\epsilon_j\xi_j})}\prod_{\substack{j\in J\\ k\notin J}}(1-e^{i(\epsilon_j\xi_j+\xi_k)})^{-1}(1-e^{i(\epsilon_j\xi_j-\xi_k)})^{-1}$$
$$\times\prod_{\substack{j,k\in J\\ j<k}}(1-e^{i(\epsilon_j\xi_j+\epsilon_k\xi_k)})^{-1}(1-qe^{i(\epsilon_j\xi_j+\epsilon_k\xi_k)})^{-1},$$

$$\hat{U}_{K,p} := (-1)^p \sum_{\substack{I\subset K,\, |I|=p\\ \epsilon_j\in\{1,-1\},\, j\in I}} \Bigg(\prod_{j\in I} \frac{\prod_{0\le r\le 3}(1-\hat{t}_r e^{i\epsilon_j\xi_j})}{(1-e^{2i\epsilon_j\xi_j})(1-qe^{2i\epsilon_j\xi_j})} \times \prod_{\substack{j\in I\\ k\in K\setminus I}} (1-e^{i(\epsilon_j\xi_j+\xi_k)})^{-1}(1-e^{i(\epsilon_j\xi_j-\xi_k)})^{-1} \times \prod_{\substack{j,k\in I\\ j<k}} (1-e^{i(\epsilon_j\xi_j+\epsilon_k\xi_k)})^{-1}(1-q^{-1}e^{-i(\epsilon_j\xi_j+\epsilon_k\xi_k)})^{-1} \Bigg)$$

(so $\hat{H}_1 = \hat{H}$). The diagonalization in Proposition 1 now generalizes to the complete system of commuting quantum integrals $\hat{H}_1, \ldots, \hat{H}_n$ as follows.

Theorem 2 (Bispectral Dual System). *Let E_l $(1 \le l \le n)$ denote the self-adjoint multiplication operator in $\ell^2(\rho_0 + \Lambda, \Delta)$ given by*

$$(E_l f)(\rho_0 + \lambda) := E_{\lambda,l} f(\rho_0 + \lambda) \qquad (\lambda \in \Lambda) \tag{6.5a}$$

(on the domain of $f \in \ell^2(\rho_0 + \Lambda, \Delta)$ for which $\langle E_l f, E_l f\rangle_\Delta < \infty$), where

$$E_{\lambda,l} := q^{-\lambda_1-\lambda_2\cdots-\lambda_{l-1}}(q^{-\lambda_l}-1) + t_0^2 q^{-\lambda_1-\lambda_2\cdots-\lambda_{n-1}}(q^{\lambda_n}-1)\delta_{n-l}. \tag{6.5b}$$

The q-difference operators $\hat{H}_l$ (6.4) constitute nonnegative unbounded self-adjoint operators with purely discrete spectra in $L^2(\mathbb{A}, \hat{\Delta} d\xi)$ that are simultaneously diagonalized by the (inverse) deformed hyperoctahedral q-Whittaker transform $\boldsymbol{F}$ (4.6a), (4.6b):

$$\hat{H}_l = \boldsymbol{F} \circ E_l \circ \boldsymbol{F}^{-1}, \qquad l = 1, \ldots, n. \tag{6.5c}$$

Proof. It suffices to verify that

$$\hat{H}_l p_\lambda = E_{\lambda,l} p_\lambda \quad (\lambda \in \Lambda,\ l = 1, \ldots, n).$$

This is achieved by multiplying the lth eigenvalue equation in Eq. (5.8) of [D3] by a scaling factor $t^{l(n-l)+l(l-1)/2}$ and performing the limit $t \to 0$. Indeed, since the Macdonald–Koornwinder polynomial $\mathbf{p}_\lambda$ converges to the deformed hyperoctahedral q-Whittaker function p_λ, we see from the explicit formulas for the operators in question that the LHS of the cited eigenvalue equation converges in this limit manifestly to $\hat{H}_l p_\lambda$ (up to an overall factor t_0^l). Hence, the RHS must also have a finite limit for $t \to 0$, which confirms that p_λ is an eigenfunction of $\hat{H}_l$ (using again that $\mathbf{p}_\lambda \xrightarrow{t\to 0} p_\lambda$). For $l > 1$ it is not obvious from [D3, Eq. (5.5)] that the (limiting) eigenvalue is indeed given by $E_{\lambda,l}$ (6.5b), but this can be deduced quite easily from the asymptotics of m_λ and $\hat{H}_l m_\lambda$ at $\xi = -ci\rho$, $\rho := (n, n-1, \ldots, 2, 1)$ for $c \to +\infty$. Indeed, one readily computes that for $c \to +\infty$: $m_\lambda = e^{\langle\lambda,\rho\rangle c}(1 + o(1))$ and $\hat{H}_l m_\lambda = E_{\lambda,l} e^{\langle\lambda,\rho\rangle c}(1 + o(1))$ (using the explicit formula for $\hat{H}_l$ and the asymptotics

$$\frac{\prod_{0\le r\le 3}(1-\hat{t}_r e^{i\epsilon\xi_j})}{(1-e^{2i\epsilon\xi_j})(1-qe^{2i\epsilon\xi_j})} \xrightarrow{c\to+\infty} \begin{cases} t_0^2 & \text{if } \epsilon = 1 \\ 1 & \text{if } \epsilon = -1 \end{cases} \qquad (1 \le j \le n)$$

and

$$(1 - q^a e^{i\epsilon(\xi_j \pm \xi_k)})^{-1} \overset{c\to+\infty}{\longrightarrow} \begin{cases} 0 & \text{if } \epsilon = 1 \\ 1 & \text{if } \epsilon = -1 \end{cases} \qquad (1 \leq j < k \leq n),$$

where $a \in \{1, 0, -1\}$). But then also $p_\lambda = e^{\langle\lambda,\rho\rangle c}(1+o(1))$ and $\hat{H}_l p_\lambda = E_{\lambda,l} e^{\langle\lambda,\rho\rangle c}(1+o(1))$ for $c \to +\infty$ by the triangularity (3.3a) and the property that $\langle\mu, \rho\rangle < \langle\lambda, \rho\rangle$ if $\mu < \lambda$. The upshot is that the eigenvalue of $\hat{H}_l$ on the eigenpolynomial p_λ must be equal to $E_{\lambda,l}$. □

The q-difference operators $\hat{H}_l$ (6.4) commute in the space of W-invariant trigonometric polynomials on $\mathbb{T}$. It is clear from Theorem 2 that this commutativity extends in the Hilbert space in the resolvent sense: for

$$z_l \notin \sigma(\hat{H}_l) := \{E_{\lambda,l} \mid \lambda \in \Lambda\} \subset [0, +\infty) \qquad (l = 1, \ldots, n)$$

the resolvents $(\hat{H}_1 - z_1\mathrm{I})^{-1}, \ldots, (\hat{H}_n - z_n\mathrm{I})^{-1}$ of the unbounded operators $\hat{H}_1, \ldots, \hat{H}_n$ mutually commute as bounded operators in $L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$.

Theorem 2 and Sect. 5 lift the bispectral duality of H (4.7) and $\hat{H}$ (6.2a),(6.2b) to the complete systems of commuting quantum integrals. The bispectral dual integrable system $\hat{H}_1, \ldots, \hat{H}_n$ associated with our difference Toda chain can actually be identified as the strong-coupling limit ($t = q^g$, $g \to +\infty$) of a trigonometric Ruijsenaars-type difference Calogero-Moser system with hyperoctahedral symmetry [D2]. Analogous bispectral dual systems were linked previously to the open quantum Toda chain and Ruijsenaars' open difference Toda chain. Specifically, the open quantum Toda chain and the strong-coupling limit of Ruijsenaars' rational difference Calogero-Moser system turn out to be bispectral duals of each other [B,HR,Sk2,Kz], and the same holds true for Ruijsenaars' open difference Toda chain and the $t = 0$ trigonometric/hyperbolic Ruijsenaars-Macdonald operators [GLO1,HR,BC]. Dualities of this type were actually first established for the corresponding particle systems within the realms of classical mechanics: the action-angle transforms linearizing the open Toda chain and the strong-coupling limit of the rational Ruijsenaars-Schneider system are the inverses of each other and the same holds true for the action-angle transforms for Ruijsenaars' open relativistic Toda chain and the strong-coupling limit of the hyperbolic Ruijsenaars-Schneider system [R1,F].

7. Parameter Reductions

As already anticipated at the end of Sect. 2, for $\hat{t}_2 = -\hat{t}_3 = q^{1/2}$ and $\hat{t}_0 = -\hat{t}_1 \to 1$ (so $t_0 = -t_1 \to 1$ and $t_2 = -t_3 \to q^{1/2}$) the difference Toda Hamiltonian H (4.7) and the deformed hyperoctahedral q-Whittaker functions $p_\lambda(\xi)$, $\lambda \in \Lambda$ degenerate to a difference Toda Hamiltonian and q-Whittaker functions of type D_n [Su1,KT,E,S, C]. Even though formally these limiting values of the parameters do not respect our restriction that $\hat{t}_r \in (-1, 1)\backslash\{0\}$ (for $r = 0, \ldots, 3$), it is readily inferred from the formulas that the results of Sects. 3–6 nevertheless remain valid at this specialization of the parameters.

In this section we are concerned with the behavior for $\hat{t}_0 \to 0$. In this limit, the difference Toda chain turns out to be governed by a Hamiltonian of the form

$$\begin{aligned}\mathrm{H} = T_1 &+ \sum_{j=2}^{n}(1 - q^{x_{j-1}-x_j})T_j + \sum_{j=1}^{n-1}(1 - q^{x_j - x_{j+1}})T_j^{-1} \\ &+ \left(\prod_{1\le r<s\le 3}(1 - \hat{t}_r\hat{t}_s q^{x_n - 1})\right)(1 - q^{x_n})T_n^{-1} \\ &+ (\hat{t}_1 + \hat{t}_2 + \hat{t}_3)q^{x_n} + \hat{t}_1\hat{t}_2\hat{t}_3 q^{2x_n}(q^{x_{n-1}-x_n} + q^{-x_n - 1} - 1 - q^{-1}).\end{aligned} \tag{7.1}$$

When $\hat{t}_3 = 0$, the Hamiltonian in question constitutes a Ruijsenaars-type difference counterpart of the quantum Toda chain with one-sided boundary potentials of Morse type [Sk1,I]. If in addition $\hat{t}_2 = -1$, then the difference Toda chain under consideration amounts to a quantization of a relativistic Toda chain with boundary potentials introduced by Suris [Su1,KT]. For $\hat{t}_1 = \hat{t}_2 = \hat{t}_3 = 0$ and for $\hat{t}_1 = -\hat{t}_2 = q^{1/2}$ with $\hat{t}_3 = -1$, we recover in turn hyperoctahedral difference Toda chains of type B_n and C_n that are diagonalized by q-Whittaker functions of type C_n and B_n, respectively [E,S,C]. Again, even though formally none of these specializations respect our restriction that $\hat{t}_r \in (-1, 1)\setminus\{0\}$ (for $r = 1, 2, 3$), it is clear that the formulas below in fact do remain valid.

7.1. Deformed hyperoctahedral q-Whittaker function. For $\hat{t}_0 \to 0$, the deformed hyperoctahedral q-Whittaker functions $p_\lambda(\xi)$ (3.3a), (3.3b) degenerate into a three-parameter family of orthogonal polynomials $\mathrm{p}_\lambda(\xi)$, $\lambda \in \Lambda$ associated with the weight function

$$\hat{\Delta}(\xi) = \frac{1}{(2\pi)^n}\prod_{1\le j<k\le n}\left|(e^{i(\xi_j+\xi_k)}, e^{i(\xi_j-\xi_k)})_\infty\right|^2 \prod_{1\le j\le n}\left|\frac{(e^{2i\xi_j})_\infty}{\prod_{1\le r\le 3}(\hat{t}_r e^{i\xi_j})_\infty}\right|^2.$$

The orthogonality relations for these polynomials read [cf. Eq. (4.5)]

$$\int_{\mathbb{A}} \mathrm{p}_\lambda(\xi)\overline{\mathrm{p}_\mu(\xi)}\,\hat{\Delta}(\xi)\mathrm{d}\xi = \begin{cases}\Delta_\lambda^{-1} & \text{if } \lambda = \mu, \\ 0 & \text{otherwise,}\end{cases} \tag{7.2}$$

where

$$\Delta_\lambda = \frac{\Delta_0}{(q)_{\lambda_n}\prod_{1\le r<s\le 3}(\hat{t}_r\hat{t}_s)_{\lambda_n}}\prod_{1\le j<n}\frac{1}{(q)_{\lambda_j-\lambda_{j+1}}}$$

with

$$\Delta_0 = (q)_\infty \prod_{1\le r<s\le 3}(\hat{t}_r\hat{t}_s)_\infty.$$

For $n = 1$, the limit $p_\lambda \overset{\hat{t}_0\to 0}{\longrightarrow} \mathrm{p}_\lambda$ amounts to a well-known reduction from the Askey-Wilson polynomials to the continuous dual q-Hahn polynomials [KLS].

7.2. Hamiltonian. The difference Toda eigenvalue equation $H\psi_\xi = \hat{E}(\xi)\psi_\xi$ becomes in the limit $\hat{t}_0 \to 0$ of the form $\mathrm{H}\phi_\xi = \hat{E}(\xi)\phi_\xi$ with $\phi_\xi : \Lambda \to \mathbb{C}$ given by $\phi_\xi(\lambda) = \mathrm{p}_\lambda(\xi)$ ($\xi \in \mathbb{A}, \lambda \in \Lambda$), where H (7.1) acts on $f : \Lambda \to \mathbb{C}$ via

$$(\mathrm{H}f)(\lambda) = \sum_{\substack{1\le j\le n\\ \lambda+e_j\in\Lambda}} v_j^+(\lambda)f(\lambda+e_j) + \sum_{\substack{1\le j\le n\\ \lambda-e_j\in\Lambda}} v_j^-(\lambda)f(\lambda-e_j) + u(\lambda)f(\lambda), \qquad (7.3)$$

with

$$v_j^+(\lambda) = (1-q^{\lambda_{j-1}-\lambda_j}),$$
$$v_j^-(\lambda) = (1-q^{\lambda_j-\lambda_{j+1}})\Big((1-q^{\lambda_n})\prod_{1\le r<s\le 3}(1-\hat{t}_r\hat{t}_s q^{\lambda_n-1})\Big)^{\delta_{n-j}},$$
$$u(\lambda) = (\hat{t}_1+\hat{t}_2+\hat{t}_3)q^{\lambda_n} + \hat{t}_1\hat{t}_2\hat{t}_3 q^{2\lambda_n}(q^{\lambda_{n-1}-\lambda_n} + q^{-\lambda_n-1} - 1 - q^{-1})$$

(subject to the convention that $\lambda_0 = +\infty$ and $\lambda_{n+1} = -\infty$).

7.3. Diagonalization and integrability. Let $\mathbf{F} : \ell^2(\Lambda,\Delta) \to L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$ denote the ($\hat{t}_0 \to 0$ degenerate) Hilbert space isomorphism determined by the orthogonal basis p_λ, $\lambda \in \Lambda$:

$$(\mathbf{F}f)(\xi) = \langle f, \phi_\xi\rangle_\Delta = \sum_{\lambda\in\Lambda} f(\lambda)\overline{\phi_\xi(\lambda)}\Delta_\lambda \qquad (7.4a)$$

($f \in \ell^2(\Lambda,\Delta)$) with

$$(\mathbf{F}^{-1}\hat{f})(\lambda) = \langle \hat{f}, \overline{\phi(\lambda)}\rangle_{\hat{\Delta}} = \int_A \hat{f}(\xi)\phi_\xi(\lambda)\hat{\Delta}(\xi)\mathrm{d}\xi \qquad (7.4b)$$

($\hat{f} \in L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$), and let $\hat{E}_l : L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi) \to L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$ ($l = 1,\ldots,n$) be the multiplication operators defined in accordance with Sect. 5.

The commuting bounded self-adjoint operators $\mathrm{H}_1,\ldots,\mathrm{H}_n$ (with absolutely continuous spectra) in $\ell^2(\Lambda,\Delta)$ given by

$$\mathrm{H}_l = \mathbf{F}^{-1}\circ\hat{E}_l\circ\mathbf{F}, \qquad l = 1,\ldots,n, \qquad (7.5)$$

constitute a complete system of quantum integrals for the difference Toda Hamiltonian $\mathrm{H}_1 = \mathrm{H}$ (7.3).

7.4. Bispectral dual system. Let $\hat{\mathrm{H}}_1,\ldots,\hat{\mathrm{H}}_n$ denote the commuting q-difference operators in Eq. (6.4) with $\hat{t}_0 = 0$ and let $\mathrm{E}_1,\ldots,\mathrm{E}_n$ be the self-adjoint multiplication operators in $\ell^2(\Lambda,\Delta)$ given by [cf. Eqs. (6.5a), (6.5b)]

$$(\mathrm{E}_l f)(\lambda) = \mathrm{E}_{\lambda,l}f(\lambda) \qquad (\lambda\in\Lambda,\ l = 1,\ldots,n) \qquad (7.6a)$$

(on the domain of $f \in \ell^2(\Lambda,\Delta)$ for which $\langle \mathrm{E}_l f, \mathrm{E}_l f\rangle_\Delta < \infty$), with

$$\mathrm{E}_{\lambda,l} = q^{-\lambda_1-\lambda_2\cdots-\lambda_{l-1}}(q^{-\lambda_l}-1). \qquad (7.6b)$$

Then one has that

$$\hat{\mathrm{H}}_l = \mathbf{F}\circ\mathrm{E}_l\circ\mathbf{F}^{-1}, \qquad l = 1,\ldots,n, \qquad (7.7)$$

i.e. the q-difference operators constitute nonnegative unbounded self-adjoint operators with purely discrete spectra in $L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi)$ that are simultaneously diagonalized by the three-parameter (inverse) deformed hyperoctahedral q-Whittaker transform $\mathbf{F}$ (7.4a), (7.4b).

8. Scattering

In Ref. [D4] the scattering operator for a wide class of quantum lattice models was determined by stationary-phase methods originating from Ref. [R4]. It follows from the diagonalization in Theorem 1 that our difference Toda chains fit within this class of lattice models. Indeed, the deformed hyperoctahedral q-Whittaker functions p_λ, $\lambda \in \Lambda$ belong to the family of orthogonal polynomials defined in [D4, Sec. 2], since the orthogonality weight function $\hat{\Delta}(\xi)$ (3.4b) is of the indicated form (with $R = BC_n$) and moreover meets the demanded analyticity requirements. We will close by briefly indicating how the general scattering results from Ref. [D4, Sec. 4.2] specialize in the present difference Toda setting.

Let $\mathcal{H}_0$ be the self-adjoint discrete Laplacian in $\ell^2(\Lambda)$ of the form

$$(\mathcal{H}_0 f)(\lambda) := \sum_{\substack{1\le j\le n\\ \lambda+e_j\in\Lambda}} f(\lambda+e_j) + \sum_{\substack{1\le j\le n\\ \lambda-e_j\in\Lambda}} f(\lambda-e_j) \qquad (f\in\ell^2(\Lambda)),$$

and let $\mathcal{H}$ denote the pushforward

$$\mathcal{H} := \boldsymbol{\Delta}^{1/2} H \boldsymbol{\Delta}^{-1/2} \tag{8.1}$$

of the difference Toda Hamiltonian H (4.7) onto the Hilbert space $\ell^2(\Lambda)$ via the Hilbert space isomorphism $\boldsymbol{\Delta}^{1/2} : \ell^2(\rho_0+\Lambda, \Delta) \to \ell^2(\Lambda)$ given by

$$(\boldsymbol{\Delta}^{1/2} f)(\lambda) := \Delta_\lambda^{1/2} f(\rho_0+\lambda) \qquad (f\in\ell^2(\rho_0+\Lambda,\Delta)) \tag{8.2}$$

(where $\boldsymbol{\Delta}^{-1/2} := (\boldsymbol{\Delta}^{1/2})^{-1}$). Clearly, one has by Theorem 1 that

$$\mathcal{H} = \boldsymbol{\mathcal{F}}^{-1}\hat{E}\boldsymbol{\mathcal{F}} \quad \text{with} \quad \boldsymbol{\mathcal{F}} := \hat{\boldsymbol{\Delta}}^{1/2}\boldsymbol{F}\boldsymbol{\Delta}^{-1/2}, \tag{8.3}$$

where $\hat{\boldsymbol{\Delta}}^{1/2} : L^2(\mathbb{A}, \hat{\Delta}\mathrm{d}\xi) \to L^2(\mathbb{A})$ denotes the Hilbert space isomorphism given by

$$(\hat{\boldsymbol{\Delta}}^{1/2}\hat{f})(\xi) := \hat{\Delta}^{1/2}(\xi)\hat{f}(\xi) \qquad (\hat{f}\in L^2(\mathbb{A},\hat{\Delta}\mathrm{d}\xi)) \tag{8.4}$$

(and $\hat{E}$ (4.8b) is now regarded as a self-adjoint bounded multiplication operator in $L^2(\mathbb{A})$). Moreover, it is elementary that the spectral decomposition of the discrete Laplacian $\mathcal{H}_0$ is given by

$$\mathcal{H}_0 = \boldsymbol{\mathcal{F}}_0^{-1}\hat{E}\boldsymbol{\mathcal{F}}_0,$$

where $\boldsymbol{\mathcal{F}}_0 : \ell^2(\Lambda) \to L^2(\mathbb{A})$ denotes the Fourier isomorphism

$$(\boldsymbol{\mathcal{F}}_0 f)(\xi) := \sum_{\lambda\in\Lambda} f(\lambda)\overline{\chi_\xi(\lambda)} \tag{8.5a}$$

($f \in \ell^2(\Lambda)$) with the inversion formula

$$(\boldsymbol{\mathcal{F}}_0^{-1}\hat{f})(\lambda) = \int_{\mathbb{A}} \hat{f}(\xi)\chi_\xi(\lambda)\mathrm{d}\xi \tag{8.5b}$$

($\hat{f} \in L^2(\mathbb{A})$). Here we have employed the anti-invariant Fourier kernel

$$\chi_\xi(\lambda) := \frac{1}{(2\pi)^{n/2}\, i^{n^2}} \sum_{w \in W} \operatorname{sign}(w) e^{i\langle w(\rho+\lambda),\xi\rangle},$$

with $\operatorname{sign}(w) = \epsilon_1 \cdots \epsilon_n \operatorname{sign}(\sigma)$ for $w = (\sigma, \epsilon) \in W = S_n \ltimes \{1, -1\}^n$ and $\rho = (n, n-1, \ldots, 2, 1)$. Notice that $\mathcal{F}_0$ is recovered from $\mathcal{F}$ in the limit $q \to 0, \hat{t}_r \to 0$ ($r = 0, \ldots, 3$).

The scattering operator describing the large-times asymptotics of the difference Toda dynamics $e^{i\mathcal{H}t}$ relative to the Laplacian's reference dynamics $e^{i\mathcal{H}_0 t}$ turns out to be governed by an n-particle scattering matrix $\hat{\mathcal{S}}(\xi)$ that factorizes in two-particle pair matrices and one-particle boundary matrices:

$$\hat{\mathcal{S}}(\xi) := \prod_{1 \le j < k \le n} s(\xi_j - \xi_k) s(\xi_j + \xi_k) \prod_{1 \le j \le n} s_0(\xi_j), \tag{8.6a}$$

with

$$s(x) := \frac{(qe^{ix})_\infty}{(qe^{-ix})_\infty} \quad \text{and} \quad s_0(x) := \frac{(qe^{2ix})_\infty}{(qe^{-2ix})_\infty} \prod_{0 \le r \le 3} \frac{(\hat{t}_r e^{-ix})_\infty}{(\hat{t}_r e^{ix})_\infty}. \tag{8.6b}$$

To make the latter statement precise, let us denote by $C_0(\mathbb{A}_{\text{reg}})$ the dense subspace of $L^2(\mathbb{A})$ consisting of smooth test functions with compact support in the open dense subset $\mathbb{A}_{\text{reg}} \subset \mathbb{A}$ on which the components of the gradient

$$\nabla \hat{E}(\xi) = (-2\sin(\xi_1), \ldots, -2\sin(\xi_n)), \quad \xi \in \mathbb{A}$$

do not vanish and are all distinct in absolute value. We now define an unitary multiplication operator $\hat{\mathcal{S}} : L^2(\mathbb{A}, \mathrm{d}\xi) \to L^2(\mathbb{A}, \mathrm{d}\xi)$ via its restriction to $C_0(\mathbb{A}_{\text{reg}})$ as follows:

$$(\hat{\mathcal{S}} \hat{f})(\xi) := \hat{\mathcal{S}}(w_\xi \xi) \hat{f}(\xi) \qquad (\hat{f} \in C_0(\mathbb{A}_{\text{reg}}), \tag{8.7}$$

where $w_\xi \in W$ for $\xi \in \mathbb{A}_{\text{reg}}$ is such that the components of $w_\xi \nabla \hat{E}(\xi)$ are all positive and reordered from large to small.

Theorem 4.2 and Corollary 4.3 of Ref. [D4] then provide the following explicit formulas for the wave operators and scattering operator of our difference Toda chain.

Theorem 3 (Wave and Scattering Operators). *The operator limits*

$$\Omega^\pm := s - \lim_{t \to \pm\infty} e^{it\mathcal{H}} e^{-it\mathcal{H}_0}$$

converge in the strong $\ell^2(\Lambda)$-norm topology and the corresponding wave operators $\Omega^\pm$ intertwining the difference Toda dynamics $e^{i\mathcal{H}t}$ with the discrete Laplacian's dynamics $e^{i\mathcal{H}_0 t}$ are given by unitary operators in $\ell^2(\Lambda)$ of the form

$$\Omega^\pm = \boldsymbol{\mathcal{F}}^{-1} \circ \hat{\mathcal{S}}^{\mp 1/2} \circ \boldsymbol{\mathcal{F}}_0,$$

where the branches of the square roots are to be chosen such that

$$s(x)^{1/2} = \frac{(qe^{ix})_\infty}{|(qe^{ix})_\infty|} \quad \textit{and} \quad s_0(x)^{1/2} = \frac{(qe^{2ix})_\infty}{|(qe^{2ix})_\infty|} \prod_{0 \le r \le 3} \frac{|(\hat{t}_r e^{ix})_\infty|}{(\hat{t}_r e^{ix})_\infty}.$$

Hence, the scattering operator relating the large-times asymptotics of the difference Toda dynamics $e^{i\mathcal{H}t}$ for $t \to -\infty$ and $t \to +\infty$ is given by the unitary operator

$$\mathcal{S} := (\Omega^+)^{-1}\Omega^- = \boldsymbol{\mathcal{F}}_0^{-1} \circ \hat{\mathcal{S}} \circ \boldsymbol{\mathcal{F}}_0.$$

The degenerate case of the difference Toda chain discussed in Sect. 7 is also covered by Theorem 3, upon setting ρ_0 equal to the nulvector in Eq. (8.2), replacing H (4.7) by H (7.3) in $\mathcal{H}$ (8.1) and $\boldsymbol{F}$ (4.6a), (4.6b) by $\mathbf{F}$ (7.4a), (7.4b) in $\boldsymbol{\mathcal{F}}$ (8.3), and substituting $\hat{t}_0 = 0$ overall.

Appendix A: Macdonald–Koornwinder Polynomials

This appendix collects some key properties of the Macdonald–Koornwinder multivariate Askey-Wilson polynomials [K,D3,M]. In the case of one variable ($n = 1$), the properties below specialize to well-known formulas for the Askey-Wilson polynomials (see e.g. [KLS]).

The Macdonald–Koornwinder polynomials $\mathbf{p}_\lambda(\xi)$ ($\lambda \in \Lambda$, $\xi \in \mathbb{T}$) are defined as polynomials of the type in Eqs. (3.3a), (3.3b), (3.4a) associated with the weight function [K, Sec. 5], [M, Ch. 5.3]:

$$\hat{\boldsymbol{\Delta}}(\xi) = \frac{1}{(2\pi)^n} \prod_{1\le j\le n} \left| \frac{(e^{2i\xi_j})_\infty}{\prod_{0\le r\le 3} (\hat{t}_r e^{i\xi_j})_\infty} \right|^2 \prod_{1\le j<k\le n} \left| \frac{(e^{i(\xi_j+\xi_k)}, e^{i(\xi_j-\xi_k)})_\infty}{(te^{i(\xi_j+\xi_k)}, te^{i(\xi_j-\xi_k)})_\infty} \right|^2,$$

with $q \in (0, 1)$ and $t, \hat{t}_r \in (-1, 1)\backslash\{0\}$ ($r = 0, \ldots, 3$). For $t \to 0$ this weight function passes into that of Eq. (3.4b), whence the polynomials in question degenerate in this limit continuously to the deformed hyperoctahedral q-Whittaker functions of Sect. 3. Notice in this respect that for $x \in \mathbb{R}$ and $|t| < \varepsilon$ (< 1) quotients of the form $(e^{ix})_\infty/(te^{ix})_\infty$ remain bounded in absolute value by $(-1)_\infty/(\varepsilon)_\infty$, so we may interchange limits and integration for $t \to 0$ when integrating trigonometric polynomials against the Macdonald–Koornwinder weight function $\hat{\boldsymbol{\Delta}}(\xi)$ over the bounded alcove $\mathbb{A}$ (by dominated convergence).

The normalized Macdonald–Koornwinder polynomials

$$\mathbf{P}_\lambda(\xi) := \mathbf{c}_\lambda \mathbf{p}_\lambda(\xi) \qquad (\lambda \in \Lambda_n), \tag{A.1a}$$

where

$$\mathbf{c}_\lambda := \prod_{1\le j\le n} \frac{(\tau_j^2)_{2\lambda_j}}{\prod_{0\le r\le 3} (t_r\tau_j)_{\lambda_j}} \prod_{1\le j<k\le n} \frac{(\tau_j\tau_k)_{\lambda_j+\lambda_k}}{(t\tau_j\tau_k)_{\lambda_j+\lambda_k}} \frac{(\tau_j\tau_k^{-1})_{\lambda_j-\lambda_k}}{(t\tau_j\tau_k^{-1})_{\lambda_j-\lambda_k}} \tag{A.1b}$$

with $\tau_j := t^{n-j} t_0$ ($j = 1, \ldots, n$) and t_r ($r = 0, \ldots, 3$) given by Eq. (4.1), satisfy the following orthogonality relations [K, Sec. 5], [D3, Sec. 7], [M, Ch. 5.3]:

$$\int_{\mathbb{A}} \mathbf{P}_\lambda(\xi)\overline{\mathbf{P}_\mu(\xi)}\hat{\boldsymbol{\Delta}}(\xi)\mathrm{d}\xi = \begin{cases} \boldsymbol{\Delta}_\lambda^{-1} & \text{if } \lambda = \mu, \\ 0 & \text{otherwise,} \end{cases} \tag{A.2a}$$

with

$$\boldsymbol{\Delta}_\lambda := \boldsymbol{\Delta}_0 \prod_{1\le j\le n}\left(\frac{1-\tau_j^2 q^{2\lambda_j}}{1-\tau_j^2}\prod_{0\le r\le 3}\frac{(t_r\tau_j)_{\lambda_j}}{(qt_r^{-1}\tau_j)_{\lambda_j}}\right)$$
$$\times\prod_{1\le j<k\le n}\frac{1-\tau_j\tau_k q^{\lambda_j+\lambda_k}}{1-\tau_j\tau_k}\frac{(t\tau_j\tau_k)_{\lambda_j+\lambda_k}}{(qt^{-1}\tau_j\tau_k)_{\lambda_j+\lambda_k}}\frac{1-\tau_j\tau_k^{-1}q^{\lambda_j-\lambda_k}}{1-\tau_j\tau_k^{-1}}\frac{(t\tau_j\tau_k^{-1})_{\lambda_j-\lambda_k}}{(qt^{-1}\tau_j\tau_k^{-1})_{\lambda_j-\lambda_k}} \tag{A.2b}$$

and

$$\boldsymbol{\Delta}_0 := \prod_{1\le j\le n}\frac{(q,t^j)_\infty \prod_{0\le r<s\le 3}(\hat{t}_r\hat{t}_s t^{n-j})_\infty}{(t,\hat{t}_0\hat{t}_1\hat{t}_2\hat{t}_3 t^{2n-j-1})_\infty}. \tag{A.2c}$$

These orthogonal polynomials satisfy moreover a second-order q-difference equation [K, Sec. 5], [M, Ch. 5.3, 4.4]:

$$\mathbf{P}_\lambda(\xi)\sum_{j=1}^n\left(q^{-1}\hat{t}_0\hat{t}_1\hat{t}_2\hat{t}_3 t^{2n-1-j}(q^{\lambda_j}-1)+t^{j-1}(q^{-\lambda_j}-1)\right)$$
$$=\sum_{1\le j\le n}\hat{V}_j(\xi)\big(\mathbf{P}_\lambda(\xi-i\log(q)e_j)-\mathbf{P}_\lambda(\xi)\big)+\hat{V}_j(-\xi)\big(\mathbf{P}_\lambda(\xi+i\log(q)e_j)-\mathbf{P}_\lambda(\xi)\big), \tag{A.3}$$

with

$$\hat{V}_j(\xi) := \frac{\prod_{0\le r\le 3}(1-\hat{t}_r e^{i\xi_j})}{(1-e^{2i\xi_j})(1-qe^{2i\xi_j})}\prod_{\substack{1\le k\le n\\ k\ne j}}\frac{1-te^{i(\xi_j+\xi_k)}}{1-e^{i(\xi_j+\xi_k)}}\frac{1-te^{i(\xi_j-\xi_k)}}{1-e^{i(\xi_j-\xi_k)}},$$

and a Pieri-type recurrence formula [D3, Sec. 6], [M, Ch. 5.3, 4.4]:

$$\mathbf{P}_\lambda(\xi)\sum_{j=1}^n(2\cos(\xi_j)-\hat{\tau}_j-\hat{\tau}_j^{-1})$$
$$=\sum_{\substack{1\le j\le n\\ \lambda+e_j\in\Lambda}}V_j^+(\lambda)\left(\hat{\tau}_j\mathbf{P}_{\lambda+e_j}(\xi)-\mathbf{P}_\lambda(\xi)\right)$$
$$+\sum_{\substack{1\le j\le n\\ \lambda-e_j\in\Lambda}}V_j^-(\lambda)\left(\hat{\tau}_j^{-1}\mathbf{P}_{\lambda-e_j}(\xi)-\mathbf{P}_\lambda(\xi)\right), \tag{A.4}$$

with $\hat{\tau}_j := t^{n-j}\hat{t}_0$ $(j=1,\ldots,n)$ and

$$V_j^+(\lambda) := \frac{\hat{\tau}_1^{-1}\prod_{0\le r\le 3}(1-t_r\tau_j q^{\lambda_j})}{(1-\tau_j^2q^{2\lambda_j})(1-\tau_j^2q^{2\lambda_j+1})}\prod_{\substack{1\le k\le n\\ k\ne j}}\frac{1-t\tau_j\tau_k q^{\lambda_j+\lambda_k}}{1-\tau_j\tau_k q^{\lambda_j+\lambda_k}}\frac{1-t\tau_j\tau_k^{-1}q^{\lambda_j-\lambda_k}}{1-\tau_j\tau_k^{-1}q^{\lambda_j-\lambda_k}},$$
$$V_j^-(\lambda) := \frac{\hat{\tau}_1\prod_{0\le r\le 3}(1-t_r^{-1}\tau_j q^{\lambda_j})}{(1-\tau_j^2q^{2\lambda_j})(1-\tau_j^2q^{2\lambda_j-1})}\prod_{\substack{1\le k\le n\\ k\ne j}}\frac{1-t^{-1}\tau_j\tau_k q^{\lambda_j+\lambda_k}}{1-\tau_j\tau_k q^{\lambda_j+\lambda_k}}\frac{1-t^{-1}\tau_j\tau_k^{-1}q^{\lambda_j-\lambda_k}}{1-\tau_j\tau_k^{-1}q^{\lambda_j-\lambda_k}}$$

(where the vectors $e_1,\ldots,e_n$ refer to the standard unit basis of $\mathbb{R}^n$).

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