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Nearest-Neighbour Correlation Functions for the Supersymmetric XYZ Spin Chain and Painlevé VI

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Abstract: We study nearest-neighbour correlation functions for the ground state of the supersymmetric XYZ spin chain with odd length and periodic boundary conditions. Under a technical assumption related to the Q-operator of the corresponding eight-vertex model, we show that they can be expressed exactly in terms of the Painlevé VI tau functions s_n and $\bar{s}_n$ introduced by Bazhanov and Mangazeev. Furthermore, we give an interpretation of the correlation functions in terms of the Painlevé VI Hamiltonian.

1. Introduction

In the theory of lattice models, solvability usually refers to situations when physically relevant quantities can be computed exactly in the infinite-lattice limit. A famous example is Baxter's computation of the ground-state energy per site for the XYZ spin chain [2]. By contrast, it is much more unusual to encounter exact results for finite-size systems. In the context of the XYZ chain, one instance of this phenomenon was discovered by Stroganov [45]. Baxter had already observed that, if the model's parameters satisfy

$$J_x J_y + J_x J_z + J_y J_z = 0 \tag{1.1a}$$

and

$$J_x + J_y + J_z > 0, \tag{1.1b}$$

then the ground-state energy per site of the infinite chain takes the remarkably simple form

$$-\frac{J_x + J_y + J_z}{2}. \tag{1.2}$$

Stroganov found empirically that (1.2) seems to hold exactly also for finite chains of odd length with periodic boundary conditions.

One conceptual explanation of why the condition (1.1) is special was given by Fendley and the first author [18]. They proved that in this case the XYZ chain is supersymmetric

in the sense that, roughly speaking, the Hamiltonian can be expressed as an anticommutator of nilpotent operators. This property was used in [22] to give a rigorous proof of Stroganov's observation.

When $J_x = J_y$, the XYZ chain reduces to the XXZ chain. It is customary to take $J_x = J_y = 1$ and write $J_z = \Delta$. The condition (1.1) is then $\Delta = -1/2$. There is a large literature on the XXZ chain with $\Delta = -1/2$ and its relations to combinatorial objects such as loop configurations, plane partitions and alternating sign matrices. We mention here only the Razumov–Stroganov conjecture [36], which was eventually proved by Cantini and Sportiello [14]. Generalizing this work to the XYZ chain is difficult and relations to combinatorics are still not well understood. However, it seems that three-colourings should play a role [23,24,40].

Another intriguing aspect of the supersymmetric XYZ chain is its relations to the Painlevé VI equation, which are present even for finite chains. Bazhanov and Mangazeev studied the ground-state eigenvalue of the Q-operator, in Stroganov's setting of odd length $L = 2n+1$ and periodic boundary conditions [7,8,10]. They found that, at special values of the spectral parameter, this eigenvalue can be expressed in terms of certain polynomials denoted s_n and $\bar{s}_n$. It was observed that these polynomials satisfy recursions that can be used to identify them with tau functions of Painlevé VI. These recursions were proved in [43]. It also appears that the same polynomials are directly related to the eigenvector. In an appropriate normalization and ignoring elementary factors, its square norm is conjecturally given by $s_n s_{-n-1}$, its component with all spins equal given by s_n and its component with all but one spin equal given by $\bar{s}_n$. Partial proofs of these results have been given in [12,53].

In the present work, we study nearest-neighbour correlation functions for the ground state of the supersymmetric XYZ chain, still in Stroganov's setting. We present an overview of our results on these correlation functions in §2. We find that they can be expressed in terms of a single quantity that we denote f_n, see Proposition 2.2. In our main result, Theorem 2.3, we express f_n in terms of the combination $\bar{s}_n \bar{s}_{-n-1}/s_n s_{-n-1}$ of Painlevé tau functions. Our proof is incomplete, as it is based on a technical assumption related to the eigenvalue of the Q-operator. In Theorem 2.4, we give a more direct interpretation of f_n as a Painlevé VI Hamiltonian, evaluated at a solution of another instance of Painlevé VI, with shifted parameters.

Our methods are similar to those of Stroganov [45,46], who computed the correlation functions in the XXZ limit case, but the details are more involved. We present the details of the computation in §3. The XYZ chain can be parametrized by the crossing parameter η and the elliptic nome τ, where the supersymmetric case is $\eta = \pi/3$. Using the Hellmann–Feynman theorem, we can express the quantity f_n in terms of the ground-state energy per site ε, see (3.11). We then exploit the relation between the XYZ spin chain and the eight-vertex model to deduce an expression for f_n in terms of the transfer-matrix eigenvalue $\lambda(u)$, see Proposition 3.3. Next, we apply Baxter's TQ-relation, which relates the transfer-matrix and the Q-operator. It is at this point that we need to make an assumption, Assumption 3.4. Although Q-operators are known both for generic $\eta \neq \pi/3$ and for $\eta = \pi/3$, we do not know any Q-operator that is analytic in a neighbourhood of $\eta = \pi/3$. Thus, it is not clear that we can differentiate the TQ-relation with respect to η. However, assuming that this is allowed leads to an expression for f_n in terms of the Q-operator eigenvalue $q(u)$, see Corollary 3.8. In the case of the XXZ chain, one can write down $q(u)$ explicitly and easily finish the computation [45,46]. For the XYZ chain, most of the work remains. The key fact is a new differential-difference equation relating

$q(u)$ and $q(u + \pi)$, see Theorem 3.9. We also need some properties of the polynomials s_n and $\bar{s}_n$ proved in [43].

After having proved Theorem 2.3, we turn to Theorem 2.4 in §4. Here, the key fact is the factorization (4.2) of the Painlevé VI Hamiltonian for special parameter values, which is also related to classical solutions of Painlevé VI.

We relegate several technical points to the appendices. In "Appendix A", we collect a number of theta function identities that we use throughout the main text. "Appendix B" describes a relation between our new difference-differential equation for the Q-operator eigenvalue and the non-stationary Lamé equation of Bazhanov and Mangazeev [7]. In "Appendix C", we present several properties of the polynomials $s_n, \bar{s}_n$. Finally, we discuss a derivation of the nearest-neighbour correlation functions in the infinite-lattice limit, starting from Baxter's formula for the ground-state energy per site, in "Appendix D". It is interesting to note that our expression for f_n, given in Theorem 2.3, splits naturally as an elementary term corresponding to the infinite-lattice limit and a term involving Painlevé tau functions that gives the finite-length correction.

We conclude this introduction by mentioning several open problems. Clearly, it would be interesting to find explicit expressions for other correlation functions. For instance, the one-point correlation functions are known in the infinite-lattice limit [6,25], but an exact finite-size result for the supersymmetric case remains to be found. Another natural candidate to investigate is the finite-size emptiness formation probability, whose expression is explicitly known for the limit of the XXZ chain at $\Delta = -1/2$ [13].

One major obstruction to studying the supersymmetric XYZ chain seems to be that its ground-state eigenvectors are not known explicitly. By contrast, in the XXZ case one can write down integral formulas for all their components [38]. Importantly for many applications, these formulas extend to the inhomogeneous six-vertex model. If one had similar expressions for the eight-vertex model, one could presumably complete the proof of many properties of the ground state described in [10,12,37,53]. They might also be useful for proving our Assumption 3.4 and for computing more general correlation functions. We mention in this context the paper [20], which contains integral formulas of the desired type for the eight-vertex-solid-on-solid model.

One important limit of the supersymmetric XYZ chain is obtained by letting n and τ/i tend to infinity with $e^{\pi \mathrm{i} \tau} \sim n^{-2/3}$ [7]. This limit is believed to be related to the sine-Gordon model at its supersymmetric point and to polymers on a cylinder [19,28]. In this limit, Painlevé VI should degenerate to Painlevé III. It would be interesting to compute the corresponding limit of the correlation functions.

The present work provides further examples of the relation between the supersymmetric XYZ spin chain and the Painlevé VI equation discovered in [8]. We stress that we have no conceptual explanation for this relation. Both our incomplete proof that the polynomials s_n and $\bar{s}_n$ appear in the correlation functions and the proof that they are Painlevé tau functions [43] emerge like miracles at the end of long computations.

Another phenomenon that calls for further explanation is the relation between the classical and quantum versions of Painlevé VI. To discuss this, let us first recall the elliptic form of Painlevé VI, given in [30] as

$$\frac{d^2 q}{d\tau^2} = -\frac{1}{4\pi^2} \sum_{j=0}^{3} \beta_j \wp'(q + \omega_j | 1, \tau), \tag{1.3}$$

where $\wp$ is the Weierstrass elliptic function, β_j areparameters and

$$(\omega_0, \omega_1, \omega_2, \omega_3) = \left(0, \frac{1}{2}, \frac{\tau}{2}, \frac{\tau+1}{2}\right).$$

Writing $\tau = 2\pi i t$, it is equivalent to the Hamiltonian system

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q},$$

where

$$H = \frac{p^2}{2} - V(q, t)$$

and

$$V(q, t) = \sum_{j=0}^{3} \beta_j \wp(q + \omega_j | 1, 2\pi i t) \tag{1.4}$$

is the Darboux–Treibich–Verdier potential [16,49,50].

The corresponding Schrödinger equation (in imaginary time)

$$\psi_t = \frac{1}{2}\psi_{xx} - V(x, t)\psi \tag{1.5}$$

has been called the quantum Painlevé VI equation. There is a direct link between classical and quantum Painlevé VI based on Lax pairs, the so called quantum Painlevé–Calogero correspondence [52], see also [15,33,47,48].

In [7], it was found that the Q-operator eigenvalue satisfies the non-stationary Lamé equation, which is the special case of (1.5) where $\beta_0 = \beta_1 = n(n+1)/2$ and $\beta_2 = \beta_3 = 0$. More generally, in [43] the second author constructed solutions to (1.5) with any values $\beta_j = k_j(k_j+1)/2$, $k_j \in \mathbb{Z}$. For such parameters, the potential (1.4) has the so-called finite-gap property [49,50]. Specializing the variable x to a half-period, the resulting functions of τ are tau functions of classical Painlevé VI in the Picard class, that is, $\beta_j = l_j^2/2$, $l_j \in \mathbb{Z}$. This link between quantum and classical Painlevé VI seems different from the quantum Painlevé–Calogero correspondence of [52]. It would be interesting to know if there is a hidden connection.

2. Statement of Results

2.1. Nearest-neighbour correlation functions. We write $V = \mathbb{C}|\uparrow\rangle \oplus \mathbb{C}|\downarrow\rangle$. The Pauli matrices acting on V are

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The XYZ spin chain is defined by the Hamiltonian

$$\mathbf{H} = -\frac{1}{2}\sum_{j=1}^{L}\left(J_x\,\sigma_j^x\sigma_{j+1}^x + J_y\,\sigma_j^y\sigma_{j+1}^y + J_z\,\sigma_j^z\sigma_{j+1}^z\right) \tag{2.1}$$

acting on $V^{\otimes L}$. Here, J_x, J_y and J_z are real anisotropy parameters and the lower indices of the Pauli matrices indicate on which tensor factor they act. We will only consider periodic boundary conditions, that is, the index $L + 1$ should be understood as 1. Moreover, we will always assume that L is odd and write $L = 2n + 1$.

We are interested in the supersymmetric case (1.1). We write the lowest eigenvalue of $\mathbf{H}$ as $L\varepsilon$, where ε is the ground-state energy per site. As was mentioned in the introduction, it is known that

$$\varepsilon = -\frac{J_x + J_y + J_z}{2}. \tag{2.2}$$

Let Ψ be an eigenvector of $\mathbf{H}$ with eigenvalue $L\varepsilon$. We write

$$\langle \mathbf{A} \rangle = \frac{\langle \Psi | \mathbf{A} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

for the expectation value of an observable $\mathbf{A}$ with respect to the corresponding ground-state. Here, $\langle \Phi | \Phi' \rangle$ denotes the standard Hermitian scalar product of two vectors $\Phi, \Phi' \in V^{\otimes L}$. We are interested in the nearest-neighbour correlation functions

$$C^x = \langle \sigma_j^x \sigma_{j+1}^x \rangle, \qquad C^y = \langle \sigma_j^y \sigma_{j+1}^y \rangle, \qquad C^z = \langle \sigma_j^z \sigma_{j+1}^z \rangle. \tag{2.3}$$

Lemma 2.1. *The correlation functions* (2.3) *are independent of the choice of ground-state vector* Ψ, *as well as of the index* j.

Proof. Write $V^{\otimes L} = W^+ \oplus W^-$, where W^+ and W^- are spanned by states with, respectively, an even and an odd number of down spins. This decomposition is preserved by $\mathbf{H}$. It is proved in [22] that the ground-state eigenspace of $\mathbf{H}\big|_{W^+}$ is one-dimensional. Let Ψ^+ be a vector in this space, normalized so that $\langle \Psi^+ | \Psi^+ \rangle = 1$. Then, the whole eigenspace is spanned by Ψ^+ and $\Psi^- = \mathbf{F}\Psi^+ \in W^-$, where $\mathbf{F} = \prod_{j=1}^{L} \sigma_j^x$ is the spin-flip operator. Let $\Psi = \alpha \Psi^+ + \beta \Psi^-$ be an arbitrary ground-state vector. By orthogonality,

$$\langle \Psi | \Psi \rangle = |\alpha|^2 \langle \Psi^+ | \Psi^+ \rangle + |\beta|^2 \langle \Psi^- | \Psi^- \rangle = |\alpha|^2 + |\beta|^2.$$

Moreover, for $a \in \{x, y, z\}$,

$$\begin{aligned}
\langle \Psi | \sigma_j^a \sigma_{j+1}^a | \Psi \rangle &= |\alpha|^2 \langle \Psi^+ | \sigma_j^a \sigma_{j+1}^a | \Psi^+ \rangle + |\beta|^2 \langle \Psi^- | \sigma_j^a \sigma_{j+1}^a | \Psi^- \rangle \\
&= (|\alpha|^2 + |\beta|^2) \langle \Psi^+ | \sigma_j^a \sigma_{j+1}^a | \Psi^+ \rangle,
\end{aligned}$$

where we used in the first step that the operator $\sigma_j^a \sigma_{j+1}^a$ preserves the spaces $W^\pm$ and in the second step that it commutes with $\mathbf{F}$. This shows that the correlation functions (2.3) do not change if we replace Ψ by Ψ^+. The final statement follows since Ψ^+ is translation invariant [22] (or, alternatively, since by the first statement we could replace Ψ^+ by any one of its translates). $\qquad\square$

Our goal is to compute the correlation functions (2.3) exactly. As a first step, we express them in terms of a single quantity that we denote f_n. It will be convenient to introduce the normalized discriminant

$$Z = \frac{(J_x - J_y)^2 (J_y - J_z)^2 (J_x - J_z)^2}{J_x^2 J_y^2 J_z^2} = -4\frac{(J_x + J_y + J_z)^3}{J_x J_y J_z} - 27, \tag{2.4}$$

where the second equality depends on (1.1).

Proposition 2.2. *For the supersymmetric periodic XYZ spin chain of odd length $L = 2n + 1$, we can write*

$$C^a = 1 + \frac{J_x J_y J_z}{J_a^2 (J_x + J_y + J_z)} f_n, \qquad a \in \{x, y, z\}, \tag{2.5}$$

where f_n is a rational function of Z.

For small n, it is straightforward to compute the ground-state eigenvectors of the supersymmetric XYZ Hamiltonian and infer f_n. To give some examples, we find for $n = 0, \ldots, 5$ the expressions

$$
\begin{aligned}
f_0 &= 0, \\
f_1 &= 1, \\
f_2 &= \frac{Z + 27}{Z + 25}, \\
f_3 &= \frac{(Z + 24)(Z + 27)}{(Z + 21)(Z + 28)}, \\
f_4 &= \frac{Z^3 + 74Z^2 + 1807Z + 14520}{Z^3 + 72Z^2 + 1701Z + 13068}, \\
f_5 &= \frac{(Z + 27)(Z^4 + 96Z^3 + 3420Z^2 + 53404Z + 306735)}{(Z^2 + 44Z + 429)(Z^3 + 77Z^2 + 1991Z + 17303)}.
\end{aligned}
$$

Since the correlation functions only depend on the Hamiltonian up to normalization, we may use the parametrization

$$J_x = 1 + \zeta, \qquad J_y = 1 - \zeta, \qquad J_z = \frac{\zeta^2 - 1}{2}. \tag{2.6}$$

Then, (2.5) takes the form

$$C^x = 1 - \frac{(1 - \zeta)^2 f_n}{\zeta^2 + 3}, \quad C^y = 1 - \frac{(1 + \zeta)^2 f_n}{\zeta^2 + 3}, \quad C^z = 1 - \frac{4 f_n}{\zeta^2 + 3}, \tag{2.7}$$

where f_n is a function of

$$Z = \frac{\zeta^2 (\zeta^2 - 9)^2}{(\zeta^2 - 1)^2}. \tag{2.8}$$

The symmetry of Z under permutations of the anisotropy parameters corresponds to the fact that $Z(\zeta) = Z(\zeta')$ if and only if $\zeta' \in \{\pm\zeta, \pm\gamma, \pm\delta\}$, where

$$\gamma = \frac{\zeta + 3}{\zeta - 1}, \qquad \delta = \frac{\zeta - 3}{\zeta + 1}.$$

That is,

$$f_n(\pm\zeta) = f_n(\pm\gamma) = f_n(\pm\delta). \tag{2.9}$$

Indeed, it is easy to check that the transformations $\zeta \mapsto \zeta'$ permute the parameters (2.6) up to normalization.

2.2. Correlation functions and tau functions. Our main result gives an explicit formula for f_n in terms of the polynomials s_n and $\bar{s}_n$ introduced by Bazhanov and Mangazeev [7]. As was conjectured in [8] and proved in [43], they can be identified with tau functions of Painlevé VI and, hence, satisfy a Toda-type recursion. For $s_n = s_n(z)$, $n \in \mathbb{Z}$, this recursion takes the form

$$8(2n+1)^2 s_{n+1} s_{n-1} + 2z(z-1)(9z-1)^2 (s_n'' s_n - (s_n')^2) + 2(3z-1)^2(9z-1)s_n s_n'$$
$$-\big(4(3n+1)(3n+2) + n(5n+3)(9z-1)\big)s_n^2 = 0 \tag{2.10}$$

with starting values $s_0 = s_1 = 1$. To obtain $\bar{s}_n$, one should replace $n(5n+3)$ by $(n-1)(5n+4)$ and the starting values by $\bar{s}_0 = 1, \bar{s}_1 = 3$. It was conjectured in [31] that, in a certain natural normalization of the eigenvector Ψ, its square norm is essentially given by $s_n(\zeta^{-2})s_{-n-1}(\zeta^{-2})$. A partial proof of this conjecture is given in [53]. Thus, it is natural to expect this product in the denominator of f_n. More surprisingly, it appears that the numerator can be expressed in terms of $\bar{s}_n \bar{s}_{-n-1}$. Although we have checked the following result for chains up to length $L = 11$, we have only proved it under a technical assumption that will be explained below.

Theorem 2.3. *If* Assumption *3.4 holds, then*

$$f_n = \frac{(\zeta^2+3)(\zeta^2-3)}{(\zeta^2-1)^2} - \frac{2\zeta^2(\zeta^2+3)}{(2n+1)^2(\zeta^2-1)^2}\frac{\bar{s}_n(\zeta^{-2})\bar{s}_{-n-1}(\zeta^{-2})}{s_n(\zeta^{-2})s_{-n-1}(\zeta^{-2})}. \tag{2.11}$$

By (2.9), one can obtain seemingly different expressions for f_n by replacing ζ in (2.11) with γ or δ.

The decomposition of f_n into two terms has a natural interpretation. Namely, in "Appendix D" we argue that $f_\infty = \lim_{n\to\infty} f_n$ is given by

$$f_\infty = \begin{cases} \dfrac{(\zeta^2+3)(\zeta^2-3)}{(\zeta^2-1)^2}, & |\zeta| \geq 3, \\[2ex] \dfrac{(\delta^2+3)(\delta^2-3)}{(\delta^2-1)^2} = -\dfrac{(\zeta^2+3)(\zeta^2+6\zeta-3)}{8(\zeta-1)^2}, & -3 \leq \zeta \leq 0, \\[2ex] \dfrac{(\gamma^2+3)(\gamma^2-3)}{(\gamma^2-1)^2} = -\dfrac{(\zeta^2+3)(\zeta^2-6\zeta-3)}{8(\zeta+1)^2}, & 0 \leq \zeta \leq 3. \end{cases} \tag{2.12}$$

Hence, when $|\zeta| \geq 3$, the first term in (2.11) gives the infinite-lattice limit and the second term the finite length correction. The variants of (2.11) with ζ replaced by γ and δ have a similar interpretation in the other parameter regimes. In "Appendix D", we deduce (2.12) from Baxter's formula for the ground-state energy per site in the infinite-lattice limit. We do not know how to prove (2.12) directly from (2.11). In Fig. 1, we illustrate the convergence of f_n to f_∞.

To see that Theorem 2.3 gives the correct result for the XXZ chain, we replace ζ by γ in (2.11) and let $\zeta = 0, \gamma = -3$. Then, the parameters (2.6) reduce to $J_x = J_y = 1$, $J_z = -1/2$. At the corresponding value $z = 1/9$, the recursion (2.10) for s_n reduces to

$$2(2n+1)^2 s_{n+1}s_{n-1} = (3n+1)(3n+2)s_n^2$$

and the recursion for $\bar{s}_n$ is identical. It easily follows that $\bar{s}_n(1/9) = 3^n s_n(1/9)$. This leads to $f_n = 9/8 - 9/(8L^2)$ and we recover Stroganov's results [45,46]:

$$C^x = C^y = \frac{5}{8} + \frac{3}{8L^2}, \qquad C^z = -\frac{1}{2} + \frac{3}{2L^2}.$$
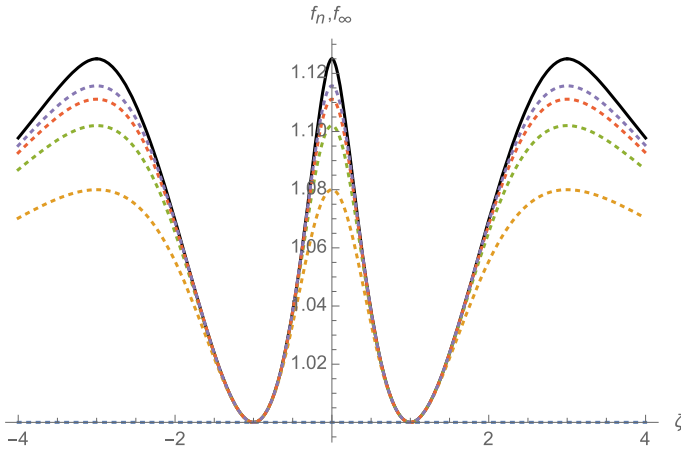
Fig. 1. Plots of f_n for $n = 1, \ldots, 5$ (dotted lines) and f_∞ (black solid line) as functions of ζ

One can also verify Theorem 2.3 in the limit $\zeta \to \infty$, which corresponds to $J_x = J_y = 0$ and $J_z = 1/2$ (after rescaling the Hamiltonian appropriately). Indeed, it follows from [41, Thm. 4.1] that $s_n(0) \neq 0$ for all n, $\bar{s}_n(0) \neq 0$ for $n \geq 0$ and that $\bar{s}_{-n-1}(z)$ is divisible by z^n for $n > 0$. Hence, the second term in (2.11) tends to zero (except when $n = 0$) and we obtain $C^x = C^y = 0$, $C^z = 1$. This is trivial to check directly since the ground-state vector can be chosen as $\Psi = |\uparrow\rangle^{\otimes L}$.

2.3. The Painlevé Hamiltonian.

The expression (2.11) can be interpreted as the Painlevé VI Hamiltonian, evaluated at a solution to the same equation with different parameters. To explain this, we recall the algebraic form of Painlevé VI,

$$\frac{d^2q}{dt^2} = \frac{1}{2}\left(\frac{1}{q} + \frac{1}{q-1} + \frac{1}{q-t}\right)\left(\frac{dq}{dt}\right)^2 - \left(\frac{1}{t} + \frac{1}{t-1} + \frac{1}{q-t}\right)\frac{dq}{dt}$$
$$+ \frac{q(q-1)(q-t)}{t^2(t-1)^2}\left(\alpha + \beta\frac{t}{q^2} + \gamma\frac{t-1}{(q-1)^2} + \delta\frac{t(t-1)}{(q-t)^2}\right). \tag{2.13}$$

As in [32], we will write

$$\alpha = \frac{\alpha_1^2}{2}, \qquad \beta = -\frac{\alpha_4^2}{2}, \qquad \gamma = \frac{\alpha_3^2}{2}, \qquad \delta = \frac{1 - \alpha_0^2}{2}$$

and introduce α_2 so that

$$\alpha_0 + \alpha_1 + 2\alpha_2 + \alpha_3 + \alpha_4 = 1. \tag{2.14}$$

There is a change of variables that takes (2.13) to the elliptic form (1.3), where the correspondence of parameters is

$$(\beta_0, \beta_1, \beta_2, \beta_3) = \left(\frac{\alpha_1^2}{2}, \frac{\alpha_4^2}{2}, \frac{\alpha_3^2}{2}, \frac{\alpha_0^2}{2}\right).$$

With

$$p = \frac{1}{2}\left(\frac{\alpha_4}{q} + \frac{\alpha_3}{q-1} + \frac{\alpha_0 - 1}{q-t} + \frac{t(t-1)}{q(q-1)(q-t)}\frac{dq}{dt}\right),$$

the Painlevé equation (2.13) is equivalent to the non-stationary Hamiltonian system [29]

$$t(t-1)\frac{dq}{dt} = \frac{\partial H}{\partial p}, \qquad t(t-1)\frac{dp}{dt} = -\frac{\partial H}{\partial q}, \tag{2.15}$$

where

$$H = q(q-1)(q-t)p^2 - \{(\alpha_0-1)q(q-1) + \alpha_3 q(q-t) + \alpha_4(q-1)(q-t)\}p$$
$$+ \alpha_2(\alpha_1+\alpha_2)(q-t).$$

Starting from one solution of Painlevé VI, one can obtain further solutions by applying Bäcklund transformations [34]. For instance, if (q, p) solves (2.15), then

$$T(q) = \frac{tp(pq-\alpha_4)}{(pq+\alpha_2)(pq+\alpha_1+\alpha_2)} \tag{2.16}$$

defines another solution with shifted parameters

$$T(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) = (\alpha_0-1, \alpha_1, \alpha_2+1, \alpha_3-1, \alpha_4).$$

We will apply this transformation to the algebraic solution (q_0, p_0) with

$$\alpha_0 = \alpha_1 = \alpha_3 = \alpha_4 = 0, \qquad \alpha_2 = \frac{1}{2},$$

defined by the parametrization

$$q_0 = \frac{s(s+2)}{2s+1}, \qquad p_0 = -\frac{2s+1}{2(s-1)(s+2)}, \qquad t = \frac{s(s+2)^3}{(2s+1)^3}. \tag{2.17}$$

We can then give the following curious interpretation of the function f_n.

Theorem 2.4. *The expression* (2.11) *can be written as*

$$f_n = \frac{(s^2+s+1)(s^2+4s+1)}{(s+1)^4} - \frac{4(2s+1)^3(s^2+4s+1)}{(2n+1)^2 s(s+1)^4}\left(H' + \frac{(2n+1)^2}{4}t\right),$$

where t is as in (2.17)*,*

$$Z = \frac{(s-1)^4(s+2)(2s+1)}{s(s+1)^4}, \tag{2.18}$$

and where $H' = H'(q_n, p_n, t)$ is the Painlevé VI Hamiltonian with parameters

$$(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) = \left(\frac{1}{2} - n, 0, \frac{1}{2} + n, -\frac{1}{2} - n, 0\right), \tag{2.19}$$

evaluated at $(q_n, p_n) = T^n(q_0, p_0)$, which solves Painlevé VI with parameters

$$(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) = \left(-n, 0, \frac{1}{2} + n, -n, 0\right).$$

To write Theorem 2.4 in terms of the parametrization (2.6) one should equate (2.8) and (2.18). This is a sextic equation, whose solutions can be written

$$\frac{(s+2)(2s+1)}{s} \in \{\zeta^2, \gamma^2, \delta^2\}. \tag{2.20}$$

Theorem 2.4 holds with each of the corresponding six choices for s.

3. Computation of the Correlation Functions

3.1. The eight-vertex model. To compute f_n, we will exploit the relation between the XYZ spin chain and the eight-vertex model [2]. With respect to the basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ of $V^{\otimes 2}$, the R-matrix of the eight-vertex model is given by

$$R = \begin{bmatrix} a & 0 & 0 & d \\ 0 & b & c & 0 \\ 0 & c & b & 0 \\ d & 0 & 0 & a \end{bmatrix},$$

where a, b, c, d are Boltzmann weights. The transfer-matrix is the operator on $V^{\otimes L}$ defined by

$$\mathbf{T} = \mathrm{Tr}_0(R_{01} R_{02} \cdots R_{0L}),$$

where the index 0 refers to an additional auxiliary copy of V. The parameter combinations

$$\zeta = \frac{cd}{ab}, \qquad \Gamma = \frac{a^2 + b^2 - c^2 - d^2}{2ab} \tag{3.1}$$

play a special role. Indeed, if (a', b', c', d') is another set of parameters such that $\zeta' = \zeta$ and $\Gamma' = \Gamma$, then the corresponding transfer-matrices $\mathbf{T}$ and $\mathbf{T}'$ commute.

An important step in Baxter's solution of the eight-vertex model is to parametrize the Boltzmann weights by theta functions. In our conventions,

$$a = \rho\,\theta_4(2\eta|2\tau)\theta_4(u - \eta|2\tau)\theta_1(u + \eta|2\tau), \tag{3.2a}$$
$$b = \rho\,\theta_4(2\eta|2\tau)\theta_1(u - \eta|2\tau)\theta_4(u + \eta|2\tau), \tag{3.2b}$$
$$c = \rho\,\theta_1(2\eta|2\tau)\theta_4(u - \eta|2\tau)\theta_4(u + \eta|2\tau), \tag{3.2c}$$
$$d = \rho\,\theta_1(2\eta|2\tau)\theta_1(u - \eta|2\tau)\theta_1(u + \eta|2\tau); \tag{3.2d}$$

see (A.1) for the definition of Jacobi theta functions. The spectral parameter u and the crossing parameter η can be taken as complex, and the modular parameter τ as complex in the upper half-plane. Without loss of generality, we fix the normalization ρ as

$$\rho = \frac{2}{\theta_2(0|\tau)\theta_4(0|2\tau)},$$

which implies

$$a + b = \frac{\theta_1(2\eta|\tau)}{\theta_1(\eta|\tau)}\theta_1(u|\tau). \tag{3.3}$$

As a function of u, the transfer-matrix satisfies the quasi-periodicity and reflection symmetry

$$\mathbf{T}(u + \pi) = \mathbf{T}(-u) = (-1)^L \mathbf{T}(u), \qquad \mathbf{T}(u + \pi\tau) = (-1)^L e^{-iL(2u+\pi\tau)}\mathbf{T}(u). \tag{3.4}$$

In the parametrization (3.2), the quantities (3.1) are independent of u. More precisely [37, Eqs. (2.6)–(2.7)],

$$\zeta = \frac{\theta_1(2\eta|2\tau)^2}{\theta_4(2\eta|2\tau)^2}, \qquad \Gamma = \frac{\theta_2(2\eta|2\tau)\theta_3(2\eta|2\tau)\theta_4(0|2\tau)^2}{\theta_2(0|2\tau)\theta_3(0|2\tau)\theta_4(2\eta|2\tau)^2}. \tag{3.5}$$

Hence, the transfer-matrices $\mathbf{T}(u)$ form a commuting family for fixed η and τ. Moreover, the XYZ Hamiltonian is contained within this family in the sense that

$$\mathbf{H} = \frac{L(a_u + c_u)}{2b_u} \text{ Id} - \frac{a}{b_u} \mathbf{T}^{-1}\mathbf{T}_u \Big|_{u=\eta}, \tag{3.6}$$

where the subscripts denote u-derivatives and the parameters are related through

$$J_x = 1 + \zeta, \qquad J_y = 1 - \zeta, \qquad J_z = \Gamma. \tag{3.7}$$

As was noted by Baxter [2], when $\eta = \pi/3$ the supersymmetry condition (1.1) holds. That is, $\Gamma = (\zeta^2 - 1)/2$ and we recover (2.6).

Let us choose $\Psi = \Psi^+$ as in the proof of Lemma 2.1. It belongs to the sector W^+ spanned by states with an even number of down spins. Since W^+ is preserved by $\mathbf{H}$, the ground-state eigenvalue of $\mathbf{H}\big|_{W^+}$ remains single on W^+ for η near $\pi/3$. We will still denote this eigenvalue by $L\varepsilon$, where we know from (2.2) that

$$\varepsilon\Big|_{\eta=\pi/3} = -\frac{(\zeta^2 + 3)}{4}. \tag{3.8}$$

We extend Ψ to an eigenvector that depends analytically on η. It is also an eigenvector of the transfer-matrices $\mathbf{T}(u)$; the eigenvalue will be denoted λ. It was conjectured in [45] and proved in [22] that

$$\lambda\Big|_{\eta=\pi/3} = \theta_1(u|\tau)^L. \tag{3.9}$$

For generic η, there are no simple finite-size expressions for neither ε nor λ, but (3.6) gives the relation

$$\varepsilon = \frac{a_u + c_u}{2b_u} - \frac{a}{Lb_u} \frac{\lambda_u}{\lambda}\Big|_{u=\eta}. \tag{3.10}$$

3.2. Proof of Proposition 2.2. We will now prove that Proposition 2.2 holds, with

$$f_n = \frac{\varepsilon(2\varepsilon_\eta + \Gamma_\eta)}{\zeta\zeta_\eta - \Gamma_\eta}\Big|_{\eta=\pi/3}, \tag{3.11}$$

where the subscripts on the right-hand side denote η-derivatives.

We first note that (2.1) implies

$$L\varepsilon = \langle \mathbf{H} \rangle = -\frac{L}{2}\left(J_x C^x + J_y C^y + J_z C^z\right). \tag{3.12}$$

The Hellmann–Feynman theorem asserts that, if $\mathbf{H}$ depends smoothly on a parameter, then

$$\langle \mathbf{H} \rangle' = \langle \mathbf{H}' \rangle,$$

where the prime denotes the derivative with respect to the parameter. Thus, we can write

$$\varepsilon' = -\frac{1}{2}\left(J_x' C^x + J_y' C^y + J_z' C^z\right).$$

The derivative may be taken with respect to either η or τ. Together with (3.12), we thus obtain a system of three linear equations for C^x, C^y and C^z. Consider this system at the point $\eta = \pi/3$. Using (3.7) and (3.8), it can be written

$$
\begin{bmatrix} 1+\zeta & 1-\zeta & \frac{1}{2}(\zeta^2 - 1) \\ \zeta_\eta & -\zeta_\eta & \Gamma_\eta \\ 1 & -1 & \zeta \end{bmatrix} \begin{bmatrix} C^x \\ C^y \\ C^z \end{bmatrix} = \begin{bmatrix} \frac{1}{2}(\zeta^2 + 3) \\ -2\varepsilon_\eta \\ \zeta \end{bmatrix}. \tag{3.13}
$$

The determinant of the coefficient matrix in (3.13) is $2(\Gamma_\eta - \zeta\zeta_\eta)$. By Lemma A.2,

$$
\zeta\zeta_\eta - \Gamma_\eta \Big|_{\eta=\pi/3} = 6\chi \frac{a}{b_u} \Big|_{u=\eta=\pi/3}, \tag{3.14}
$$

where

$$
\chi = \frac{\theta_1'(0|\tau)^2 \theta_2(\pi/3|\tau)^2}{\theta_1(\pi/3|\tau)^2 \theta_2(0|\tau)^2}. \tag{3.15}
$$

This expression implies, in particular, that the determinant is non-zero for generic τ. It is then easy to see that (3.13) has the unique solution (2.7), where f_n is given by (3.11). As we have noted, (2.7) can equivalently be written as (2.5).

It remains to show that f_n is a rational function of Z. Note that the eigenvalue equation for Ψ is a linear system whose coefficients are linear in (J_x, J_y, J_z). Hence, we may normalize Ψ so that its coefficients are homogeneous polynomials in the anisotropy parameters. Then, (2.5) defines f_n as a homogeneous rational function of J_x, J_y and J_z. To complete the proof we need the following fact.

Lemma 3.1. *Permuting the anisotropy parameters entails a corresponding permutation of the correlation functions. That is, if $(\tilde{x}, \tilde{y}, \tilde{z})$ is any permutation of the symbols (x, y, z) and we consider the correlations as functions of the anisotropy parameters, then*

$$
C^a(J_{\tilde{x}}, J_{\tilde{y}}, J_{\tilde{z}}) = C^{\tilde{a}}(J_x, J_y, J_z), \qquad a \in \{x, y, z\}. \tag{3.16}
$$

Proof. Let $\tilde{\mathbf{H}}$ be the operator obtained from the Hamiltonian $\mathbf{H}$ after replacing the parameters (J_x, J_y, J_z) with $(J_{\tilde{x}}, J_{\tilde{y}}, J_{\tilde{z}})$. It is well-known that there exists $U \in SU(2)$ such that $\sigma^a = \pm U \sigma^{\tilde{a}} U^{-1}$, $a \in \{x, y, z\}$. The signs involved in these formulas will be irrelevant. Writing $\mathbf{U} = U^{\otimes L}$, we have $\tilde{\mathbf{H}} = \mathbf{U}\mathbf{H}\mathbf{U}^{-1}$. Given a ground-state eigenvector Ψ of $\mathbf{H}$, we can obtain a ground-state eigenvector of $\tilde{\mathbf{H}}$ as $\mathbf{U}\Psi$. By Lemma 2.1, we may use $\mathbf{U}\Psi$ to compute the left-hand side of (3.16). That is, we are reduced to the identity

$$
\frac{\langle \mathbf{U}\Psi | \sigma_j^a \sigma_{j+1}^a | \mathbf{U}\Psi \rangle}{\langle \mathbf{U}\Psi | \mathbf{U}\Psi \rangle} = \frac{\langle \Psi | \sigma_j^{\tilde{a}} \sigma_{j+1}^{\tilde{a}} | \Psi \rangle}{\langle \Psi | \Psi \rangle},
$$

which is clear from the properties of U. $\qquad\square$

It is easy to see that the expressions (2.5) are consistent with Lemma 3.1 only if f_n is invariant under permutation of the anisotropy parameters. It must then be a rational expression in $e_1 = J_x + J_y + J_z$, $e_2 = J_x J_y + J_x J_z + J_y J_z$ and $e_3 = J_x J_y J_z$. Since $e_2 = 0$ and f_n is homogeneous, it is in fact a function of e_1^3/e_3 or, equivalently, of Z. This completes the proof of Proposition 2.2.

3.3. Expressions in terms of the transfer-matrix eigenvalue. The next step is to express (3.11) in terms of the transfer-matrix eigenvalue λ.

Lemma 3.2. *One has*

$$\varepsilon_\eta + \frac{\Gamma_\eta}{2}\bigg|_{\eta=\pi/3} = -\frac{a}{Lb_u}\frac{\lambda_{u\eta}\lambda - \lambda_u\lambda_\eta}{\lambda^2}\bigg|_{u=\eta=\pi/3}. \tag{3.17}$$

Proof. Since $a = c$ and $b = d = 0$ when $u = \eta$, the case $u \to \eta$ of (3.1) is

$$\Gamma = \frac{a_u - c_u}{b_u}\bigg|_{u=\eta}.$$

Combining this with (3.10) gives

$$\varepsilon + \frac{\Gamma}{2} = \frac{a_u}{b_u} - \frac{a}{Lb_u}\frac{\lambda_u}{\lambda}\bigg|_{u=\eta}.$$

Writing the variables as (u, η), we split this expression as $T_1 + T_2$, where

$$T_1 = \frac{a_u}{b_u}(\eta, \eta) - \frac{a}{Lb_u}(\eta, \eta)\frac{\lambda_u}{\lambda}(\eta, \pi/3),$$

$$T_2 = \frac{a}{Lb_u}(\eta, \eta)\left(\frac{\lambda_u}{\lambda}(\eta, \pi/3) - \frac{\lambda_u}{\lambda}(\eta, \eta)\right).$$

By (3.3) and (3.9),

$$\frac{\lambda_u}{\lambda}(u, \pi/3) = L\frac{a_u + b_u}{a + b}(u, \eta),$$

where η on the right-hand side is arbitrary. In particular, taking $u = \eta$ and using that $b(\eta, \eta) = 0$ gives

$$\frac{\lambda_u}{\lambda}(\eta, \pi/3) = L\frac{a_u + b_u}{a}(\eta, \eta).$$

It follows that $T_1 = -1$. Hence, the only contribution to (3.17) comes from T_2. To give a non-zero contribution, the derivative must hit the second factor and we obtain

$$\frac{\partial T_2}{\partial \eta}\bigg|_{\eta=\pi/3} = -\frac{a}{Lb_u}\frac{\partial}{\partial \eta}\frac{\lambda_u}{\lambda}\bigg|_{u=\eta=\pi/3},$$

which equals the right-hand side of (3.17). □

Using also (3.8) and (3.14), we may now rewrite (3.11) as follows.

Proposition 3.3. *The quantity f_n appearing in (2.7) can be expressed as*

$$f_n = \frac{\zeta^2 + 3}{12L\chi}\frac{\lambda_{u\eta}\lambda - \lambda_u\lambda_\eta}{\lambda^2}\bigg|_{u=\eta=\pi/3}.$$

3.4. The TQ-relation. Let

$$\phi(u) = \lambda(u)\Big|_{\eta=\pi/3} = \theta_1(u|\tau)^L.$$

We have reduced the computation of the correlation functions to the evaluation of

$$\lambda_{u\eta}\lambda - \lambda_u\lambda_\eta\Big|_{u=\eta=\pi/3} = \lambda_{u\eta}\phi - \phi_u\lambda_\eta\Big|_{u=\eta=\pi/3}.$$

To handle the η-derivatives, we will exploit Baxter's TQ-relation.

A Q-operator is a family of operators $\mathbf{Q} = \mathbf{Q}(u)$ (depending also on η and τ) acting on $V^{\otimes L}$ such that $\mathbf{Q}(u)$ and $\mathbf{T}(v)$ always commute, and

$$\mathbf{T}(u)\mathbf{Q}(u) = \phi(u - \eta)\mathbf{Q}(u + 2\eta) + \phi(u + \eta)\mathbf{Q}(u - 2\eta).$$

It is also natural to assume the quasi-periodicity and reflection symmetry

$$\mathbf{Q}(u + 2\pi) = \mathbf{Q}(-u) = \mathbf{Q}(u), \qquad \mathbf{Q}(u + 2\pi\tau) = e^{-2iL(u+\pi\tau)}\mathbf{Q}(u),$$

which are consistent with (3.4).

Baxter gave two different constructions of Q-operators for the eight-vertex model. Unfortunately, neither of these work in our situation, that is, for odd L and $\eta = \pi/3$. Baxter's first Q-operator [1] is defined in terms of the inverse of an auxiliary operator $\mathbf{Q}_R$, which is not invertible for $\eta = \pi/3$. His second definition [3] only works for even L. Different constructions due to Fabricius [17] and Roan [39], give solutions defined at $\eta = \pi/3$, but as we also need the η-derivative at $\eta = \pi/3$, that is not enough for our purposes. One possible way out of this problem was suggested by Bazhanov and Mangazeev [7]. They propose that the ground-state eigenvector Ψ belongs to a subspace of $V^{\otimes L}$ where $\mathbf{Q}_R$ is invertible. Restricting Baxter's first Q-operator $\mathbf{Q}$ to that space, one would then have $\mathbf{Q}\Psi = Q\Psi$, where the eigenvalue $Q = Q(u)$ satisfies

$$\lambda(u)Q(u) = \phi(u - \eta)Q(u + 2\eta) + \phi(u + \eta)Q(u - 2\eta), \tag{3.18a}$$

$$Q(u + 2\pi) = Q(-u) = Q(u), \qquad Q(u + 2\pi\tau) = e^{-2iL(u+\pi\tau)}Q(u). \tag{3.18b}$$

Our results will be derived from these identities, which still lack a rigorous proof. More formally, we make the following assumption:

Assumption 3.4. There exists a non-zero function Q that satisfies (3.18) and is analytic for all $u \in \mathbb{C}$, $\text{Im}(\tau) > 0$ and η in some neighbourhood of $\pi/3$ (that may depend on u and τ).

Lemma 3.5. *If* Assumption 3.4 *holds, then the space of functions satisfying the conditions described there is two-dimensional. It is spanned by two functions $Q^\pm$ that satisfy*

$$Q^\pm(u + \pi) = Q^\mp(u), \qquad Q^\pm(u + \pi\tau) = \pm e^{-iL(u+\pi\tau/2)}Q^\pm(u). \tag{3.19}$$

Moreover, writing $Q^\pm = Q^\pm(u|\tau)$, these functions can be normalized so that

$$Q^\pm(u|\tau + 2) = Q^\mp(u|\tau). \tag{3.20}$$

Proof. By (3.4), the transfer-matrix eigenvalue $\lambda(u)$ obeys

$$\lambda(u + \pi) = -\lambda(u), \qquad \lambda(u + \pi\tau) = -e^{-\mathrm{i}L(2u+\pi\tau)}\lambda(u),$$

and we also have

$$\phi(u + \pi) = -\phi(u), \qquad \phi(u + \pi\tau) = -e^{-\mathrm{i}L(2u+\pi\tau)}\phi(u).$$

Using these relations, it is easy to check that if $Q(u)$ solves (3.18), then so do $Q(u + \pi)$ and $e^{\mathrm{i}L(u+\pi\tau/2)}Q(u + \pi\tau)$. We can then write any solution as $Q = \tilde{Q}_+ + \tilde{Q}^-$, where

$$\tilde{Q}^\pm(u) = \frac{1}{2}\left(Q(u) \pm e^{\mathrm{i}L(u+\pi\tau/2)}Q(u + \pi\tau)\right).$$

If Q is non-zero, the functions $\tilde{Q}^\pm$ cannot both vanish identically. If $\tilde{Q}^+ \not\equiv 0$, we let $Q^+ = \tilde{Q}^+$ and define $Q^-(u) = Q^+(u + \pi)$. Otherwise, we let $Q^- = \tilde{Q}^-$ and $Q^+(u) = Q^-(u + \pi)$. It is then clear that $Q^\pm$ satisfy (3.18) and (3.19).

We will write $q(u) = Q^+(u)|_{\eta=\pi/3}$. This function satisfies

$$\phi(u)q(u) + \phi\left(u + \frac{2\pi}{3}\right)q\left(u + \frac{2\pi}{3}\right) + \phi\left(u - \frac{2\pi}{3}\right)q\left(u - \frac{2\pi}{3}\right) = 0, \quad \text{(3.21a)}$$

$$q(u + 2\pi) = q(-u) = q(u), \qquad q(u + \pi\tau) = e^{-\mathrm{i}L(u+\pi\tau/2)}q(u). \quad \text{(3.21b)}$$

It is proved in [41] that the space of entire functions subject to these conditions is one-dimensional. (More precisely, it follows from the discussion in [41, §5.4] that this is a consequence of [41, Thm. 2.4].) Since a small perturbation cannot increase the dimension of the solution space, our assumption that a non-zero Q exists implies that Q^+ remains unique for η near $\pi/3$. In particular, the function $\tilde{Q}^+$ is proportional to Q^+ and similarly $\tilde{Q}^-$ is proportional to Q^-. Hence, any solution Q is in the span of Q^+ and Q^-.

For the final statement, we first note that $Q^-(u|\tau + 2) = Q^+(\pi - u|\tau + 2)$ satisfies the properties defining Q^+, so there exists $f(\tau)$ (depending also on η) such that

$$Q^+(\pi - u|\tau + 2) = f(\tau)Q^+(u|\tau).$$

In particular, $u = \pi/2$ has the same multiplicity as a zero of both $Q^+(u|\tau + 2)$ and $Q^+(u|\tau)$. If k is this multiplicity and $a(\tau)$ is the leading Taylor coefficient of $Q^+(u|\tau)$ at $u = \pi/2$, then

$$f(\tau) = \lim_{u\to\pi/2}\frac{Q^+(\pi - u|\tau + 2)}{Q^+(u|\tau)} = (-1)^k\frac{a(\tau + 2)}{a(\tau)}.$$

It is now easy to check that, if k is even, then the renormalized functions $\tilde{Q}^\pm = Q^\pm/a$ satisfy $\tilde{Q}^\pm(u|\tau + 2) = \tilde{Q}^\mp(u|\tau)$. If k is odd, one can instead take $\tilde{Q}^\pm = e^{\mathrm{i}\pi\tau/2}Q^\pm/a$. $\square$

From now on, we fix two functions $Q^\pm$ satisfying all conditions in Lemma 3.5. Writing, as in the proof, $q = Q^+|_{\eta=\pi/3}$, we have in particular

$$q(u + \pi|\tau) = q(u|\tau + 2). \quad \text{(3.22)}$$

The functions $Q^\pm$ satisfy the Wronskian relations [9]

$$Q^+(u - \eta)Q^-(u + \eta) - Q^+(u + \eta)Q^-(u - \eta) = W\phi(u), \quad \text{(3.23a)}$$

$$Q^+(u - 2\eta)Q^-(u + 2\eta) - Q^+(u + 2\eta)Q^-(u - 2\eta) = W\lambda(u), \qquad (3.23b)$$

where $W = W(\eta, \tau)$ is independent of u. We introduce the difference operator

$$(\mathbf{R}f)(\tau) = f(\tau) - f(\tau + 2).$$

Using (3.20), we can then write (3.23) more compactly as

$$\mathbf{R}\left(Q^+(u - \eta)Q^-(u + \eta)\right) = W\phi(u), \qquad (3.24a)$$

$$\mathbf{R}\left(Q^+(u - 2\eta)Q^-(u + 2\eta)\right) = W\lambda(u). \qquad (3.24b)$$

At $\eta = \pi/3$, these relations are equivalent and simplify to

$$W\phi(u) = \mathbf{R}\left(q\left(u - \frac{\pi}{3}\right)q\left(u - \frac{2\pi}{3}\right)\right). \qquad (3.25)$$

The following lemma expresses the η-derivatives of the transfer-matrix eigenvalue in terms of derivatives of the function q alone. The expressions follow from a cancellation for which the supersymmetric value $\eta = \pi/3$ is crucial. This simple but important feature was first observed by Stroganov [45,46]. It enables the computation of the correlation functions from the TQ-relation.

Lemma 3.6. *For $\eta = \pi/3$,*

$$\frac{W\lambda_\eta}{3} = \mathbf{R}\left(q\left(u - \frac{2\pi}{3}\right)q'\left(u - \frac{\pi}{3}\right) - q'\left(u - \frac{2\pi}{3}\right)q\left(u - \frac{\pi}{3}\right)\right), \qquad (3.26a)$$

$$\frac{W\lambda_{u\eta}}{3} = \mathbf{R}\left(q\left(u - \frac{2\pi}{3}\right)q''\left(u - \frac{\pi}{3}\right) - q''\left(u - \frac{2\pi}{3}\right)q\left(u - \frac{\pi}{3}\right)\right). \qquad (3.26b)$$

Here and below, primes refer to derivatives in the spectral parameter u.

Proof. Differentiating (3.24) with respect to η gives

$$W_\eta\phi = \mathbf{R}\Big(- Q_u^+(u - \eta)Q^-(u + \eta) + Q^+(u - \eta)Q_u^-(u + \eta)$$
$$+ Q_\eta^+(u - \eta)Q^-(u + \eta) + Q^+(u - \eta)Q_\eta^-(u + \eta)\Big),$$

$$W_\eta\lambda + W\lambda_\eta = \mathbf{R}\Big(- 2Q_u^+(u - 2\eta)Q^-(u + 2\eta) + 2Q^+(u - 2\eta)Q_u^-(u + 2\eta)$$
$$+ Q_\eta^+(u - 2\eta)Q^-(u + 2\eta) + Q^+(u - 2\eta)Q_\eta^-(u + 2\eta)\Big).$$

At $\eta = \pi/3$, we may write the second relation as

$$W_\eta\phi + W\lambda_\eta = \mathbf{R}\Big(- 2Q_u^-(u + \eta)Q^+(u - \eta) + 2Q^-(u + \eta)Q_u^+(u - \eta)$$
$$+ Q_\eta^-(u + \eta)Q^+(u - \eta) + Q^-(u + \eta)Q_\eta^+(u - \eta)\Big).$$

Subtracting the first relation, all terms involving η-derivatives cancel and we obtain

$$W\lambda_\eta = 3\mathbf{R}\big(Q^-(u + \eta)Q_u^+(u - \eta) - Q_u^-(u + \eta)Q^+(u - \eta)\big).$$

This can be expressed as (3.26a), which gives (3.26b) after differentiation. $\qquad\square$

Specializing $u = \pi/3$ in (3.25) and its first two u-derivatives, as well as in (3.26), gives the following useful relations.

Corollary 3.7. *At $u = \eta = \pi/3$, the following identities hold:*

$$W\phi = \mathbf{R}\left(q(0)q\left(\frac{\pi}{3}\right)\right),$$

$$W\phi_u = -\mathbf{R}\left(q(0)q'\left(\frac{\pi}{3}\right)\right),$$

$$W\phi_{uu} = \mathbf{R}\left(q(0)q''\left(\frac{\pi}{3}\right) + q''(0)q\left(\frac{\pi}{3}\right)\right),$$

$$\frac{W\lambda_\eta}{3} = \mathbf{R}\left(q(0)\,q'\left(\frac{\pi}{3}\right)\right),$$

$$\frac{W\lambda_{u\eta}}{3} = \mathbf{R}\left(q''(0)\,q\left(\frac{\pi}{3}\right) - q(0)\,q''\left(\frac{\pi}{3}\right)\right).$$

Using these identities in Proposition 3.3 gives the following result.

Corollary 3.8. *We have*

$$f_n = -\frac{(\zeta^2 + 3)}{4L\chi\phi(\pi/3)W}\,\mathbf{R}(X), \tag{3.27}$$

where

$$X = q(0)\left(q''\left(\frac{\pi}{3}\right) + \frac{\phi'}{\phi}\left(\frac{\pi}{3}\right)q'\left(\frac{\pi}{3}\right)\right) - q''(0)q\left(\frac{\pi}{3}\right).$$

3.5. Differential relations. We will need the following difference-differential equation for $q(u)$, which may have some independent interest. Recall that the Weierstrass function $\wp(u|\tau_1, \tau_2)$ is the unique meromorphic function with period lattice $\mathbb{Z}\tau_1 + \mathbb{Z}\tau_2$ that has poles only at the lattice points and satisfies

$$\wp(u|\tau_1, \tau_2) = \frac{1}{u^2} + \mathcal{O}(u^2), \quad u \to 0. \tag{3.28}$$

Theorem 3.9. *The Q-operator eigenvalues $q(u)$ and $q(u + \pi)$ are related by*

$$\left(\frac{\partial^2}{\partial u^2} - V(u) - \alpha\right)\frac{\phi(u)q(u)}{\theta_1(3u|3\tau)^n\,\theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)} = \beta\,\frac{\theta_4\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)\phi(u)q(u + \pi)}{\theta_1(3u|3\tau)^n\,\theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2}, \tag{3.29}$$

where

$$V(u) = n(n + 1)\wp\left(u\left|\frac{\pi}{3}, \pi\tau\right.\right) + 2\wp\left(u + \pi + \frac{\pi\tau}{2}\left|\frac{2\pi}{3}, \pi\tau\right.\right)$$

and the parameters α and β are independent of u.

To prepare the proof of Theorem 3.9, let

$$f_1(u) = \theta_3\left(\frac{3u}{2}\bigg|\frac{3\tau}{2}\right)q(u), \qquad f_2(u) = f_1(u+\pi)$$

and write $\Omega = g^{-1}(\partial_u^2 - V(u))g$, where

$$g(u) = \frac{\theta_1(u|\tau)^{2n+1}}{\theta_1(3u|3\tau)^n\,\theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2}.$$

With these definitions at hand, the differential relation (3.29) takes the form $\Omega(f_1) = \alpha f_1 + \beta f_2$. To prove it, we first give an analytic description of the space Θ spanned by f_1 and f_2, and then prove that $\Omega(f_1) \in \Theta$. We remark that $\Omega(f_2) \notin \Theta$.

Lemma 3.10. *Let Θ be the space of all entire functions f that satisfy*

$$\phi(u)f(u) + \phi\left(u + \frac{2\pi}{3}\right)f\left(u + \frac{2\pi}{3}\right) + \phi\left(u - \frac{2\pi}{3}\right)f\left(u - \frac{2\pi}{3}\right) = 0, \quad (3.30\text{a})$$

$$f(u + 2\pi) = f(-u) = f(u), \qquad f(u + \pi\tau) = e^{-i(n+2)(2u+\pi\tau)}f(u). \qquad (3.30\text{b})$$

Then, Θ is spanned by f_1 and f_2.

The fact that Θ is two-dimensional is also a special case of [41, Thm. 2.4]. To make the connection, note that $f \in \Theta$ if and only if the function $(\phi f)(u)/\theta_4(3u|3\tau)$ is in the space denoted $\Theta_n^{(n,-1,-1,n)}$ in [41], where the variables (z, τ) in [41] correspond to our $(u/2\pi, \tau/2)$.

Proof of Lemma 3.10. It is straightforward to check from (3.21) that f_1, $f_2 \in \Theta$. Consider the functional $(\Lambda f)(u) = f(\pi + \pi\tau/2)$ defined on Θ. We observe that substituting $u = \pi + \pi\tau/2$ in (3.30a) and using (3.30b) gives

$$(\phi f)\left(\pi + \frac{\pi\tau}{2}\right) + 2(\phi f)\left(\pi + \frac{\pi\tau}{2} + \frac{2\pi}{3}\right) = 0.$$

This equality shows that if $f \in \text{Ker}(\Lambda)$, then f vanishes at all zeroes of $\theta_3(3u/2|3\tau/2)$. Hence, $f/\theta_3(3u/2|3\tau/2)$ is an entire function satisfying (3.21), so f is proportional to f_1.

On the other hand, it follows from [43, Thm. 2.1] that $q(\pi\tau/2) \neq 0$, so $f_2 \notin \text{Ker}(\Lambda)$. Since both the kernel and image of Λ are one-dimensional, $\dim(\Theta) = \dim \text{Ker}(\Lambda) + \dim \text{Im}(\Lambda) = 2$. $\qquad\square$

Proof of Theorem 3.9. It remains to verify that $h = \Omega f_1 \in \Theta$. It is straightforward to check that f satisfies (3.30) if and only if

$$(gf)(u) + (gf)\left(u + \frac{2\pi}{3}\right) + (gf)\left(u - \frac{2\pi}{3}\right) = 0,$$

$$(gf)(u + 2\pi) = (gf)(u), \qquad (gf)(u + \pi\tau) = (gf)(-u) = (-1)^{n+1}(gf)(u).$$

$$(3.31)$$

Since the operator $\partial_u^2 - V(u)$ preserves these conditions, we only need to check that h is an entire function.

The only possible poles of h are at the zeroes and poles of g (which include the poles of the potential V). Modulo translations by $2\pi\mathbb{Z} + \pi\tau\mathbb{Z}$ and the reflection $u \mapsto -u$, there are six such points, namely,

$$0, \quad \frac{\pi}{3}, \quad \frac{2\pi}{3}, \quad \pi, \quad \frac{\pi}{3} + \frac{\pi\tau}{2}, \quad \pi + \frac{\pi\tau}{2}. \tag{3.32}$$

It is straightforward to check that h is regular at the points (3.32). We only provide details for the point $u_0 = 2\pi/3$. It is a zero of $\theta_1(3u|3\tau)$, so $(gf_1)(u_0 + u) = \mathcal{O}(u^{-n})$. Moreover, it follows from (3.31) that

$$(gf_1)(u_0 + u) + (-1)^{n+1}(gf_1)(u_0 - u) = -(gf_1)(u).$$

Since $u = 0$ is a zero of both $\theta_1(3u|3\tau)$ and $\theta_1(u|\tau)$, $(gf_1)(u) = \mathcal{O}(u^{n+1})$. Hence,

$$(gf_1)(u_0 + u) = Au^{-n} + \mathcal{O}(u^{2-n}) + Bu^{n+1} + \mathcal{O}(u^{n+3}).$$

If $n \geq 1$, this simplifies to

$$(gf_1)(u_0 + u) = Au^{-n} + \mathcal{O}(u^{2-n}).$$

Acting with

$$\frac{\partial^2}{\partial u^2} - V(u_0 + u) = \frac{\partial^2}{\partial u^2} - \frac{n(n+1)}{u^2} + \mathcal{O}(1), \tag{3.33}$$

the coefficient of u^{-n-2} cancels, so the result is $\mathcal{O}(u^{-n})$. If $n = 0$, we have instead

$$(gf_1)(u_0 + u) = A + Bu + \mathcal{O}(u^2) = \mathcal{O}(1).$$

In this case (3.33) simplifies to $\partial_u^2 + \mathcal{O}(1)$, so the result is again $\mathcal{O}(1)$. In either case, dividing by g leads to a function regular at u_0.   □

Let Φ denote the alternant

$$\begin{aligned}
\Phi(u, v) &= f_1(u)f_2(v) - f_2(u)f_1(v) \\
&= \theta_3\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)\theta_4\left(\frac{3v}{2}\Big|\frac{3\tau}{2}\right)q(u)q(v + \pi) \\
&\quad - \theta_4\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)\theta_3\left(\frac{3v}{2}\Big|\frac{3\tau}{2}\right)q(u + \pi)q(v). \tag{3.34}
\end{aligned}$$

We note some properties of this function. Indicating also the τ-dependence, it follows from (3.22) that

$$\Phi(u, v|\tau + 2) = -\Phi(u, v|\tau). \tag{3.35}$$

The Wronskian relation (3.23a) is equivalent to

$$\Phi\left(u, u + \frac{2\pi}{3}\right) = \theta_3\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)\theta_4\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)\phi\left(u + \frac{\pi}{3}\right)W.$$

Inserting $u = \pi/3$ and using the theta function identity (A.4) gives

$$W = -\frac{\theta_2\left(0\big|\frac{3\tau}{2}\right)\Phi\left(\pi, \frac{\pi}{3}\right)}{\theta_1'\left(0\big|\frac{3\tau}{2}\right)\phi\left(\frac{\pi}{3}\right)}. \tag{3.36}$$

The following consequence of Theorem 3.9 is a key result for our purposes.

Corollary 3.11. *The Q-operator eigenvalue q satisfies*

$$(2n + 3)q''(0)q\left(\frac{\pi}{3}\right) + (2n - 1)q(0)\frac{(q\phi)''\left(\frac{\pi}{3}\right)}{\phi\left(\frac{\pi}{3}\right)} + 2(2n + 1)Eq(0)q\left(\frac{\pi}{3}\right)$$

$$= 3i\frac{q'\left(\pi + \frac{\pi\tau}{2}\right)}{q\left(\frac{\pi\tau}{2}\right)}\Phi\left(0, \frac{\pi}{3}\right), \tag{3.37}$$

where E is defined by the expansion

$$\frac{\theta_1(u|\tau)^{2n+3}}{\theta_1(3u|3\tau)^{2n}\theta_4(3u|3\tau)} = E_0 u^3 + E_0 E u^5 + \mathcal{O}(u^7). \tag{3.38}$$

Proof. We will consider (3.29) near $u = u_0$, where $u_0 = \pi + \pi\tau/2$, 0 and $\pi/3$. In the first case, u_0 is a zero of $q(u)$ and of $\theta_3(3u/2|3\tau/2)$. The only contribution to the leading term on the left-hand side comes from the singular part of the potential, which is $2(u - u_0)^{-2}$. Thus,

$$\beta = \lim_{u \to u_0} -\frac{2}{(u - u_0)^2}\frac{\theta_3\left(\frac{3u}{2}\middle|\frac{3\tau}{2}\right)q(u)}{\theta_4\left(\frac{3u}{2}\middle|\frac{3\tau}{2}\right)q(u + \pi)}.$$

We have

$$\frac{\theta_3\left(\frac{3u}{2}\middle|\frac{3\tau}{2}\right)}{\theta_4\left(\frac{3u}{2}\middle|\frac{3\tau}{2}\right)} = i\frac{\theta_1\left(\frac{3(u-u_0)}{2}\middle|\frac{3\tau}{2}\right)}{\theta_2\left(\frac{3(u-u_0)}{2}\middle|\frac{3\tau}{2}\right)} = \frac{3i}{2}\frac{\theta_1'\left(0\middle|\frac{3\tau}{2}\right)}{\theta_2\left(0\middle|\frac{3\tau}{2}\right)}(u - u_0) + \mathcal{O}((u - u_0)^3),$$

$$\frac{q(u)}{q(u + \pi)} = \frac{q'\left(\pi + \frac{\pi\tau}{2}\right)}{q(\frac{\pi\tau}{2})}(u - u_0) + \mathcal{O}((u - u_0)^3).$$

Using also (A.4) gives

$$\beta = -3i\,\theta_3\left(0\middle|\frac{3\tau}{2}\right)\theta_4\left(0\middle|\frac{3\tau}{2}\right)\frac{q'\left(\pi + \frac{\pi\tau}{2}\right)}{q\left(\frac{\pi\tau}{2}\right)}. \tag{3.39}$$

Turning to the case $u_0 = 0$, we define A_0 and A by

$$\frac{\phi(u)}{\theta_1(3u|3\tau)^n\theta_3\left(\frac{3u}{2}\middle|\frac{3\tau}{2}\right)} = A_0 u^{n+1} + A_0 A u^{n+3} + \mathcal{O}(u^{n+5}),$$

so that

$$\frac{\phi(u)q(u)}{\theta_1(3u|3\tau)^n\theta_3\left(\frac{3u}{2}\middle|\frac{3\tau}{2}\right)} = A_0 q(0)u^{n+1} + A_0\left(\frac{q''(0)}{2} + Aq(0)\right)u^{n+3} + \mathcal{O}(u^{n+5}).$$

The potential has the form

$$V(u) = \frac{n(n + 1)}{u^2} + 2C + \mathcal{O}(u^2),$$

where

$$C = \wp\left(\frac{\pi}{3} + \frac{\pi\tau}{2}\middle|\frac{2\pi}{3}, \pi\tau\right).$$

Inserting these expansions into (3.29) and picking out the coefficient of u^{n+1} gives

$$q(0)\alpha + \frac{\theta_4\left(0\big|\frac{3\tau}{2}\right)}{\theta_3\left(0\big|\frac{3\tau}{2}\right)} q(\pi)\beta = (2n+3)\big(q''(0) + 2Aq(0)\big) - 2Cq(0). \tag{3.40a}$$

In the same way, the expansion of (3.29) near $u_0 = \pi/3$ gives

$$q\left(\frac{\pi}{3}\right)\alpha + \frac{\theta_3\left(0\big|\frac{3\tau}{2}\right)}{\theta_4\left(0\big|\frac{3\tau}{2}\right)} q\left(\frac{2\pi}{3}\right)\beta$$

$$= -(2n-1)\left(\frac{(q\phi)''\left(\frac{\pi}{3}\right)}{\phi\left(\frac{\pi}{3}\right)} + 2Bq\left(\frac{\pi}{3}\right)\right) - 2Dq\left(\frac{\pi}{3}\right), \tag{3.40b}$$

where

$$\frac{1}{\theta_1(3u|3\tau)^n \theta_4\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)} = B_0 u^{-n} + B_0 B u^{2-n} + \mathcal{O}(u^{4-n})$$

and

$$D = \wp\left(\frac{\pi\tau}{2}\bigg|\frac{2\pi}{3}, \pi\tau\right).$$

We now eliminate α from the pair of equations (3.40) and insert the expression (3.39) for β. This leads to (3.37), with

$$(2n+1)E = (2n+3)A + (2n-1)B - C + D. \tag{3.41}$$

It remains to show that this agrees with (3.38).

It follows from the elementary theory of elliptic functions that

$$\wp\left(u\bigg|\frac{2\pi}{3}, \pi\tau\right) = P\frac{\theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2}{\theta_1\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2} + Q,$$

with P and Q independent of u. Substituting $u = \pi/3 + \pi\tau/2$, the first term on the right vanishes and we see that $Q = C$. Using (3.28) then gives

$$\frac{\theta_1\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2}{\theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2} = Pu^2 + PCu^4 + \mathcal{O}(u^6).$$

Replacing θ_3 by θ_4 gives a similar identity for D. Thus, the right-hand side of (3.41) is the quotient of the subleading and the leading coefficients of

$$\left(\frac{\theta_1(u|\tau)^{2n+1}}{\theta_1(3u|3\tau)^n \theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)}\right)^{2n+3} \left(\frac{1}{\theta_1(3u|3\tau)^n \theta_4\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)}\right)^{2n-1} \frac{\theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2}{\theta_4\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)^2}$$

$$= \left(\frac{\theta_1(u|\tau)^{2n+3}}{\theta_1(3u|3\tau)^{2n} \theta_3\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right) \theta_4\left(\frac{3u}{2}\big|\frac{3\tau}{2}\right)}\right)^{2n+1}.$$

Using also (A.6), we find that this quotient equals $(2n+1)E$. $\qquad\square$

3.6. Splitting of the function X. We now return to the expression (3.27). We split the function X into two parts, which will eventually correspond to the infinite-lattice limit and the finite-size correction of the correlation functions. More precisely, we write $X = X_1 + X_2$, where

$$X_1 = \frac{2n+1}{2}\left(q''\left(\frac{\pi}{3}\right)q(0) + q\left(\frac{\pi}{3}\right)q''(0)\right) + 2n\frac{\phi'}{\phi}\left(\frac{\pi}{3}\right)q'\left(\frac{\pi}{3}\right)q(0)$$
$$+ \left(\frac{2n-1}{2}\frac{\phi''}{\phi}\left(\frac{\pi}{3}\right) + (2n+1)E\right)q\left(\frac{\pi}{3}\right)q(0),$$

$$X_2 = -\frac{2n+3}{2}q''(0)q\left(\frac{\pi}{3}\right) - \frac{2n-1}{2}q(0)\frac{(q\phi)''\left(\frac{\pi}{3}\right)}{\phi\left(\frac{\pi}{3}\right)} - (2n+1)Eq(0)q\left(\frac{\pi}{3}\right)$$
$$= -\frac{3\mathrm{i}}{2}\frac{q'\left(\pi + \frac{\pi\tau}{2}\right)}{q\left(\frac{\pi\tau}{2}\right)}\Phi\left(0,\frac{\pi}{3}\right),$$

where the final expression follows from Corollary 3.11.

Using Corollary 3.7, one finds that

$$\mathbf{R}(X_1) = W\phi\left(2n\frac{\phi''}{\phi} - 2n\left(\frac{\phi'}{\phi}\right)^2 + (2n+1)E\right)\Bigg|_{u=\pi/3}.$$

By Lemma A.3, this can be simplified further to

$$\mathbf{R}(X_1) = -(2n+1)\phi\left(\frac{\pi}{3}\right)\frac{\chi(\gamma^2 - 3)W}{(\gamma+1)^2},$$

where χ is as in (3.15) and where as before $\gamma = (\zeta + 3)/(\zeta - 1)$. Using (3.22) and (3.35), it is straightforward to check that $\mathbf{R}(X_2) = 2X_2$. Hence,

$$\mathbf{R}(X) = -(2n+1)\phi\left(\frac{\pi}{3}\right)\frac{\chi(\gamma^2 - 3)W}{(\gamma+1)^2} - 3\mathrm{i}\frac{q'\left(\pi + \frac{\pi\tau}{2}\right)}{q\left(\frac{\pi\tau}{2}\right)}\Phi\left(0,\frac{\pi}{3}\right).$$

Inserting this expression and (3.36) in Corollary 3.8 gives the following result.

Lemma 3.12. *The function f_n can be expressed as*

$$f_n = \frac{(\gamma^2 - 3)(\gamma^2 + 3)}{(\gamma^2 - 1)^2} - \frac{3\mathrm{i}(\gamma^2 + 3)}{(2n+1)\chi(\gamma - 1)^2}\frac{\theta_1'\left(0|\frac{3\tau}{2}\right)}{\theta_2\left(0|\frac{3\tau}{2}\right)}\frac{\Phi\left(0,\frac{\pi}{3}\right)}{\Phi\left(\pi,\frac{\pi}{3}\right)}\frac{q'\left(\pi + \frac{\pi\tau}{2}\right)}{q\left(\frac{\pi\tau}{2}\right)}. \quad (3.42)$$

3.7. Proof of Theorem 2.3. To complete the proof of Theorem 2.3, we need to express the last term in (3.42) in terms of the polynomials s_n and $\bar{s}_n$. To keep close to the conventions of [43], we introduce the variables

$$x = x(u|\tau) = -\frac{\theta_3\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2\theta_1\left(\frac{3u}{2}|\frac{3\tau}{2}\right)\theta_4\left(\frac{u}{2}|\frac{\tau}{2}\right)}{\theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2\theta_1\left(\frac{u}{2}|\frac{\tau}{2}\right)\theta_4\left(\frac{3u}{2}|\frac{3\tau}{2}\right)},$$

$$z = z(\tau) = -\frac{\theta_2\left(0|\frac{\tau}{2}\right)\theta_3\left(\frac{\pi}{3}|\frac{\tau}{2}\right)}{\theta_3\left(0|\frac{\tau}{2}\right)\theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)}. \quad (3.43)$$

Then, our variables (u, τ, x, z) correspond to $(2\pi z, 2\tau, x, \zeta)$ from [43]. See (A.18) for the relation between the modular functions z and γ.

Let k_0, k_1, k_2, k_3 and n be integers, such that $m = 2n - \sum_j k_j \geq 0$. In [43], the second author introduced a family of rational functions $T_n^{(k_0, k_1, k_2, k_3)}(x_1, \ldots, x_m; z)$, which are symmetric in the variables x_j. They are defined by explicit determinant formulas that we do not repeat here. When $m = 0$, the variables x_j are absent. We denote this special case

$$t^{(k_0, k_1, k_2, k_3)}(z) = T_n^{(k_0, k_1, k_2, k_3)}(-; z), \qquad k_0 + k_1 + k_2 + k_3 = 2n. \qquad (3.44)$$

It follows from [41, Prop. 2.17] that the solution to (3.21) is

$$q(u) = q(u|\tau) = C_1 h(u) T_n^{(n, -1, 0, n)}(x; z),$$

where C_1 is independent of u and

$$h(u) = \theta_3\left(\frac{u}{2}\Big|\frac{\tau}{2}\right)\left(\frac{\theta_4\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)}{\theta_4\left(\frac{u}{2}\Big|\frac{\tau}{2}\right)}\right)^n.$$

We choose C_1 so that (3.22) is satisfied. (One can show that $C_1 = (z + 1)^{-3n(n-1)/2}$ works, but we will not need that fact.)

Denoting the half-periods in $2\pi\mathbb{Z} + \pi\tau\mathbb{Z}$ by

$$\gamma_0 = 0, \qquad \gamma_1 = \frac{\pi\tau}{2}, \qquad \gamma_2 = \pi + \frac{\pi\tau}{2}, \qquad \gamma_3 = \pi,$$

we have, for each $0 \leq j \leq 3$,

$$T_n^{(k_0, k_1, k_2, k_3)}(x_1, \ldots, x_{m-1}, x(\gamma_j|\tau); z) = T_n^{(k_0, k_1, k_2, k_3) + e_j}(x_1, \ldots, x_{m-1}; z), \quad (3.45)$$

where $e_0, \ldots, e_3$ are the canonical unit vectors of $\mathbb{Z}^4$. It follows that

$$q\left(\frac{\pi\tau}{2}\right) = C_1 h\left(\frac{\pi\tau}{2}\right) t^{(n, 0, 0, n)}(z) \qquad (3.46a)$$

and, since $h(\gamma_2) = 0$,

$$q'\left(\pi + \frac{\pi\tau}{2}\right) = C_1 h'\left(\pi + \frac{\pi\tau}{2}\right) t^{(n, -1, 1, n)}(z). \qquad (3.46b)$$

Next, we consider the function $f(u) = \Phi(u, \pi/3)$. It is a solution of (3.30) that satisfies the additional restriction $f(\pi/3) = 0$. It follows from [41, Prop. 2.17] that

$$f(u) = C_2 k(u) T_{n-1}^{(n, -1, -1, n-1)}(x; z),$$

where C_2 is independent of u and

$$k(u) = \frac{\theta_2\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)^2 \theta_3\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)}{\theta_2\left(\frac{u}{2}\Big|\frac{\tau}{2}\right)^2 \theta_3\left(\frac{u}{2}\Big|\frac{\tau}{2}\right)}\left(\frac{\theta_4\left(\frac{3u}{2}\Big|\frac{3\tau}{2}\right)}{\theta_4\left(\frac{u}{2}\Big|\frac{\tau}{2}\right)}\right)^{n-1}. \qquad (3.46c)$$

Applying again (3.45) gives

$$\Phi\left(0, \frac{\pi}{3}\right) = C_2 k(0) t^{(n+1, -1, -1, n-1)}(z), \qquad (3.46d)$$

$$\Phi\left(\pi, \frac{\pi}{3}\right) = C_2 k(\pi) t^{(n,-1,-1,n)}(z). \tag{3.46e}$$

Inserting the expressions (3.46) in Lemma 3.12, the factors C_j cancel and we obtain

$$
f_n = \frac{(\gamma^2 - 3)(\gamma^2 + 3)}{(\gamma^2 - 1)^2}
$$
$$
- \frac{3i(\gamma^2 + 3)}{(2n+1)\chi(\gamma - 1)^2} \frac{\theta_1'\left(0\middle|\frac{3\tau}{2}\right)}{\theta_2\left(0\middle|\frac{3\tau}{2}\right)} \frac{h'\left(\pi + \frac{\pi\tau}{2}\right)}{h\left(\frac{\pi\tau}{2}\right)} \frac{k(0)}{k(\pi)} \frac{t^{(n,-1,1,n)} t^{(n+1,-1,-1,n-1)}}{t^{(n,0,0,n)} t^{(n,-1,-1,n)}}. \tag{3.47}
$$

We prove in Lemma A.4 that

$$
\frac{1}{\chi} \frac{\theta_1'\left(0\middle|\frac{3\tau}{2}\right)}{\theta_2\left(0\middle|\frac{3\tau}{2}\right)} \frac{h'\left(\pi + \frac{\pi\tau}{2}\right)}{h\left(\frac{\pi\tau}{2}\right)} \frac{k(0)}{k(\pi)} = \frac{(-1)^{n+1} 2i(z+1)}{3(\gamma + 1)^2 (z-1)(2z+1)^{n-1}}. \tag{3.48}
$$

Moreover, it follows from (C.3) that

$$
\frac{t^{(n,-1,1,n)} t^{(n+1,-1,-1,n-1)}}{t^{(n,0,0,n)} t^{(n,-1,-1,n)}} = \frac{(-1)^{n+1} (z-1)^2 (2z+1)^n}{(2n+1)(z+1)^2} \frac{\bar{s}_n(\gamma^{-2})\bar{s}_{-n-1}(\gamma^{-2})}{s_n(\gamma^{-2})s_{-n-1}(\gamma^{-2})}.
$$

Using these identities and (A.18) in (3.47), we finally obtain

$$
f_n = \frac{(\gamma^2 + 3)(\gamma^2 - 3)}{(\gamma^2 - 1)^2} - \frac{2\gamma^2(\gamma^2 + 3)}{(2n+1)^2(\gamma^2 - 1)^2} \frac{\bar{s}_n(\gamma^{-2})\bar{s}_{-n-1}(\gamma^{-2})}{s_n(\gamma^{-2})s_{-n-1}(\gamma^{-2})}. \tag{3.49}
$$

Since we already know that f_n is invariant under interchanging γ and ζ, this proves Theorem 2.3.

4. Connection to Painlevé VI

In this section, we prove Theorem 2.4. We first briefly review some relevant technicalities. A rational solution of Painlevé VI can be identified with a homomorphism of differential fields $\mathbb{C}(q, p, t) \to \mathbb{C}(t)$, where $\mathbb{C}(q, p, t)$ is equipped with the derivation

$$
\delta = \frac{\partial H}{\partial p} \frac{\partial}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial}{\partial p} + t(t-1)\frac{\partial}{\partial t}
$$

and $\mathbb{C}(t)$ with $t(t-1)d/dt$. To consider more general solutions algebraically, one needs to work with field extensions. We follow the approach of [43], which uses a differential field $\mathcal{F}$ generated by q, p, t, u, v, $\alpha_0, \ldots, \alpha_4$ and $\tau_0, \ldots, \tau_4$. These are subject to the relations (2.14) as well as

$$
u^2 v^4 = t, \qquad u^4 v^2 = 1 - t.
$$

Thus, u and v represent choices of the roots $t^{-1/6}(1-t)^{1/3}$ and $t^{1/3}(1-t)^{-1/6}$, respectively. The elements τ_j are abstract tau functions, which represent inverse logarithmic derivatives of modified versions of the Hamiltonian. We can then identify the special solution (2.17) with a differential homomorphism $\mathbf{X} : \mathcal{F} \to \mathcal{M}$, where $\mathcal{M}$ is a field of modular functions. It satisfies

$$
\mathbf{X}(q) = \frac{s(s+2)}{2s+1}, \qquad \mathbf{X}(t) = \frac{s(s+2)^3}{(2s+1)^3},
$$

where $s = s(\tau)$ is now an element of $\mathcal{M}$. In [42] it was chosen as $s = z$, with z as in (3.43). To simplify the formulation of Theorem 2.4 we take here instead $s = -z - 1$, which corresponds to making a further modular transformation of the variable τ.

A Bäcklund transformation can be viewed algebraically as an automorphism of a differential field. One can define such transformations $T_1, \ldots, T_4$ that generate an action of the lattice $\mathbb{Z}^4$ on $\mathcal{F}$. The transformation (2.16) corresponds to $T = T_2^{-1} T_3$. We will write

$$\tau_{l_1 l_2 l_3 l_4} = T_1^{l_1} T_2^{l_2} T_3^{l_3} T_4^{l_4} \tau_0.$$

A main result of [43] is that the lattice of modular tau functions $\mathbf{X}(\tau_{l_1 l_2 l_3 l_4})$ can be identified with the lattice (3.44) of rational functions $t^{(k_0, k_1, k_2, k_3)}$.

To prove Theorem 2.4, we first note that substituting $s = -z - 1$ in (A.18) gives

$$\gamma^2 = \frac{(s + 2)(2s + 1)}{s}.$$

As we saw in (2.20), this leads to the relation (2.18) between the parameters Z and s. By (C.1) and (C.2),

$$\frac{\bar{s}_n(\gamma^{-2})\bar{s}_{-n-1}(\gamma^{-2})}{s_n(\gamma^{-2})s_{-n-1}(\gamma^{-2})} = \frac{s}{(s+2)(2s+1)^2} \frac{t^{(n,n,1,-1)}(s)t^{(n,n,-2,0)}(s)}{t^{(n,n,0,0)}(s)t^{(n,n,-1,-1)}(s)}.$$

It follows from [43, Thm. 4.2] (with the variable ζ there replaced by $-s - 1$) that

$$\frac{t^{(n,n,1,-1)}(s)t^{(n,n,-2,0)}(s)}{t^{(n,n,0,0)}(s)t^{(n,n,-1,-1)}(s)} = -\frac{4(s+2)^3(2s+1)}{s}\mathbf{X}\left(\frac{1}{v^2}\frac{\tau_{-1,-n,n,1}\tau_{1,-n,n+1,-1}}{\tau_{0,-n,n,0}\tau_{0,-n,n+1,0}}\right)$$

$$= -\frac{4(s+2)^3(2s+1)}{s}\mathbf{X}T^n\left(\frac{1}{v^2}\frac{\tau_{-1,0,0,1}\tau_{1,0,1,-1}}{\tau_{0,0,0,0}\tau_{0,0,1,0}}\right).$$

We also used that, by [42, Lemma 2.3], $Tv = v$. By definition, $\tau_{0,0,0,0} = \tau_0$ and one can check that $\tau_{0,0,1,0} = \tau_3$,

$$\tau_{-1,0,0,1} = -\frac{i\tau_0\tau_4 v}{\tau_1}(p(q-1) + \alpha_1 + \alpha_2),$$

$$\tau_{1,0,1,-1} = -\frac{i\tau_1\tau_3 v}{\tau_4 t}(pq(q-t) + \alpha_2 q + \alpha_4 t).$$

These expressions allow us to evaluate

$$\frac{1}{v^2}\frac{\tau_{-1,0,0,1}\tau_{1,0,1,-1}}{\tau_{0,0,0,0}\tau_{0,0,1,0}} = -\frac{(p(q-1) + \alpha_1 + \alpha_2)(pq(q-t) + \alpha_2 q + \alpha_4 t)}{t}. \qquad (4.1)$$

We can then rewrite (3.49) as

$$f_n = \frac{(s^2 + s + 1)(s^2 + 4s + 1)}{(s+1)^4} - \frac{4(2s+1)^3(s^2 + 4s + 1)}{(2n+1)^2 s(s+1)^4}$$

$$\times \mathbf{X}T^n(p(q-1) + \alpha_1 + \alpha_2)(pq(q-t) + \alpha_2 q + \alpha_4 t).$$

Theorem 2.4 now follows from comparing

$$\mathbf{X}T^n(p(q-1) + \alpha_1 + \alpha_2)(pq(q-t) + \alpha_2 q + \alpha_4 t)$$

$$= \left(p_n(q_n - 1) + n + \frac{1}{2} \right) \left(p_n(q_n - t) + n + \frac{1}{2} \right) q_n$$

with the observation that the Hamiltonian with the parameters (2.19) factors as

$$H' + \frac{(2n + 1)^2}{4} t = \left(p(q - 1) + n + \frac{1}{2} \right) \left(p(q - t) + n + \frac{1}{2} \right) q. \qquad (4.2)$$

We remark that factorizations such as (4.2) are related to the existence of classical solutions to Painlevé VI. In the case at hand, consider solutions such that the first factor in (4.2) vanishes. The system (2.15) then reduces to the single equation $tq' = (n+1/2)q$ and we recover the elementary solutions $q = Ct^{n+1/2}$. More generally, the expression (4.1) appears in the factorization

$$H + (\alpha_0 - 1)\alpha_3 t = (p(q - 1) + \alpha_1 + \alpha_2)(pq(q - t) + \alpha_2 q + \alpha_4 t),$$

which holds for $\alpha_1 + \alpha_2 + \alpha_3 = 0$. In this case, solutions such that the first factor vanishes can be expressed in terms of Gauss' hypergeometric function [34].

Data availability Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

Declarations

Conflict of interest The authors have no competing interests to declare that are relevant to the content of this article.

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Appendix A. Theta Function Identities

In this appendix we collect some useful theta function identities. Fixing τ in the upper half-plane and $p = e^{i\pi\tau}$, the Jacobi theta functions are defined by the Fourier series

$$\theta_1(u|\tau) = 2 \sum_{n=0}^{\infty} (-1)^n p^{(n+1/2)^2} \sin((2n + 1)u), \qquad (A.1a)$$

$$\theta_2(u|\tau) = 2 \sum_{n=0}^{\infty} p^{(n+1/2)^2} \cos((2n + 1)u), \qquad (A.1b)$$

$$\theta_3(u|\tau) = 1 + 2\sum_{n=1}^{\infty} p^{n^2} \cos(2nu), \tag{A.1c}$$

$$\theta_4(u|\tau) = 1 + 2\sum_{n=1}^{\infty}(-1)^n p^{n^2} \cos(2nu) \tag{A.1d}$$

or, equivalently, by the product expansions

$$\theta_1(u|\tau) = \mathrm{i}e^{\mathrm{i}\pi\tau/4 - \mathrm{i}u}(p^2, e^{2\mathrm{i}u}, p^2 e^{-2\mathrm{i}u}; p^2), \tag{A.2a}$$

$$\theta_2(u|\tau) = e^{\mathrm{i}\pi\tau/4 - \mathrm{i}u}(p^2, -e^{2\mathrm{i}u}, -p^2 e^{-2\mathrm{i}u}; p^2), \tag{A.2b}$$

$$\theta_3(u|\tau) = (p^2, -pe^{2\mathrm{i}u}, -pe^{-2\mathrm{i}u}; p^2), \tag{A.2c}$$

$$\theta_4(u|\tau) = (p^2, pe^{2\mathrm{i}u}, pe^{-2\mathrm{i}u}; p^2), \tag{A.2d}$$

where

$$(a_1, \ldots, a_n; p)_{\infty} = \prod_{j=0}^{\infty}(1 - a_1 p^j)\cdots(1 - a_n p^j).$$

Throughout, we use primes, such as in $\theta_1'(u|\tau)$, to indicate the u-derivatives of the theta functions.

Elementary quasi-periodicity and reflection relations, such as

$$\theta_1(u + \pi|\tau) = \theta_1(-u|\tau) = -\theta_1(u|\tau), \qquad \theta_1(u + \pi\tau|\tau) = -e^{-\mathrm{i}(2u + \pi\tau)}\theta_1(u|\tau)$$

will be taken for granted and used without comment. We will also need the modular transformation [51, §21.51]

$$\theta_4(u/\tau| - 1/\tau) = (\tau/\mathrm{i})^{1/2}e^{\mathrm{i}u^2/\pi\tau}\theta_2(u|\tau). \tag{A.3}$$

The identities

$$\theta_1'(0|\tau) = \theta_2(0|\tau)\theta_3(0|\tau)\theta_4(0|\tau), \tag{A.4}$$

$$\theta_4(0|2\tau)\theta_1(2u|2\tau) = \theta_1(u|\tau)\theta_2(u|\tau), \tag{A.5}$$

$$\theta_4(0|2\tau)\theta_4(2u|2\tau) = \theta_3(u|\tau)\theta_4(u|\tau), \tag{A.6}$$

$$\theta_2(0|\tau)\theta_1(u|\tau) = 2\theta_1(u|2\tau)\theta_4(u|2\tau), \tag{A.7}$$

$$\theta_2(0|\tau)\theta_2(u|\tau) = 2\theta_2(u|2\tau)\theta_3(u|2\tau), \tag{A.8}$$

$$\theta_1(2u|\tau) = 2\frac{\theta_1(u|\tau)\theta_2(u|\tau)\theta_3(u|\tau)\theta_4(u|\tau)}{\theta_2(0|\tau)\theta_3(0|\tau)\theta_4(0|\tau)}, \tag{A.9}$$

$$\theta_j(3u|3\tau) = \frac{(p^6; p^6)_{\infty}}{(p^2; p^2)_{\infty}^3}\theta_j(u|\tau)\theta_j\left(\frac{\pi}{3} + u\Big|\tau\right)\theta_j\left(\frac{\pi}{3} - u\Big|\tau\right), \quad 1 \le j \le 4, \tag{A.10}$$

are all easy consequences of (A.2). Specializing $u = \pi/3$ in (A.9) gives

$$\frac{\theta_2(\pi/3|\tau)\theta_3(\pi/3|\tau)\theta_4(\pi/3|\tau)}{\theta_2(0|\tau)\theta_3(0|\tau)\theta_4(0|\tau)} = \frac{1}{2}. \tag{A.11}$$

Many identities for Jacobi theta functions follow from the Weierstrass identity [51, §20.51, Ex. 5, and §21.43]:

$$\theta_1(x - y|\tau)\theta_1(x + y|\tau)\theta_1(u - v|\tau)\theta_1(u + v|\tau)$$
$$- \theta_1(x - u|\tau)\theta_1(x + u|\tau)\theta_1(y - v|\tau)\theta_1(y + v|\tau)$$
$$+ \theta_1(x - v|\tau)\theta_1(x + v|\tau)\theta_1(u - y|\tau)\theta_1(u + y|\tau) = 0. \tag{A.12}$$

For instance, specializing some arguments in this identity to $0, \pi/2, \pi/2 + \pi\tau/2$, or $\pi\tau/2$ leads to various addition formulas. A combination of such specializations with (A.5) and (A.6) allows one to derive the identities [21, §8.119]:

$$\theta_4(0|\tau)^2\theta_4(x + y|\tau)\theta_4(x - y|\tau) = \theta_4(x|\tau)^2\theta_4(y|\tau)^2 - \theta_1(x|\tau)^2\theta_1(y|\tau)^2 \tag{A.13}$$
$$= \theta_3(x|\tau)^2\theta_3(y|\tau)^2 - \theta_2(x|\tau)^2\theta_2(y|\tau)^2, \tag{A.14}$$
$$\theta_1(x + y|\tau)\theta_2(x - y|\tau) = \theta_1(2x|2\tau)\theta_4(2y|2\tau) + \theta_4(2x|2\tau)\theta_1(2y|2\tau). \tag{A.15}$$

Moreover, we need the differential identity [21, §8.199]

$$\frac{\partial}{\partial u} \frac{\theta_3(u|\tau)}{\theta_2(u|\tau)} = \frac{\theta_4(0|\tau)^2\theta_1(u|\tau)\theta_4(u|\tau)}{\theta_2(u|\tau)^2}. \tag{A.16}$$

By (3.5) with $\eta = \pi/3$, the parameter $\zeta = \zeta(\tau)$ in (2.6) is given by

$$\zeta = \frac{\theta_1(2\pi/3|2\tau)^2}{\theta_4(2\pi/3|2\tau)^2} = \frac{\theta_1(\pi/3|\tau)^2\theta_2(\pi/3|\tau)^2}{\theta_3(\pi/3|\tau)^2\theta_4(\pi/3|\tau)^2}, \tag{A.17a}$$

where the second identity follows from (A.5) and (A.6). We will also need

$$1 + \zeta = 2\frac{\theta_2(\pi/3|\tau)\theta_3(0|\tau)}{\theta_2(0|\tau)\theta_3(\pi/3|\tau)}, \tag{A.17b}$$

$$1 - \zeta = 2\frac{\theta_2(\pi/3|\tau)\theta_4(0|\tau)}{\theta_2(0|\tau)\theta_4(\pi/3|\tau)}, \tag{A.17c}$$

$$3 + \zeta = 2\frac{\theta_1(\pi/3|\tau)^2\theta_4(0|\tau)\theta_4(\pi/3|\tau)}{\theta_2(0|\tau)\theta_2(\pi/3|\tau)\theta_3(\pi/3|\tau)^2}, \tag{A.17d}$$

$$3 - \zeta = 2\frac{\theta_1(\pi/3|\tau)^2\theta_3(0|\tau)\theta_3(\pi/3|\tau)}{\theta_2(0|\tau)\theta_2(\pi/3|\tau)\theta_4(\pi/3|\tau)^2}. \tag{A.17e}$$

These can, for instance, be obtained from [40, Lemma 9.1]. As a consequence,

$$\gamma = \frac{\zeta + 3}{\zeta - 1} = -\frac{\theta_1(\pi/3|\tau)^2\theta_4(\pi/3|\tau)^2}{\theta_2(\pi/3|\tau)^2\theta_3(\pi/3|\tau)^2}.$$

Yet another application of [40, Lemma 9.1] then gives

$$\gamma^2 = \frac{(1 - z)(1 + 2z)}{1 + z}, \tag{A.18}$$

where z is as in (3.43).
We now return to the situation when η is generic.

Lemma A.1. *If J_x, J_y and J_z are given by* (3.7), *with ζ and Γ parametrized as in* (3.1), *then*

$$J_x J_y + J_x J_z + J_y J_z = 1 - \zeta^2 + 2\Gamma = \frac{\theta_1(3\eta|\tau)\theta_3(0|\tau)^4\theta_4(0|\tau)^4}{\theta_1(\eta|\tau)\theta_3(\eta|\tau)^4\theta_4(\eta|\tau)^4}. \tag{A.19}$$

Note that this implies Baxter's observation that (1.1) holds for $\eta = \pi/3$.

Proof. The application of (A.9) and (A.13) to (3.5) yields

$$1 - \zeta^2 = \frac{\theta_4(0|2\tau)^3\theta_4(4\eta|2\tau)}{\theta_4(2\eta|2\tau)^4}, \qquad 2\Gamma = \frac{\theta_4(0|2\tau)^3\theta_1(4\eta|2\tau)}{\theta_4(2\eta|2\tau)^3\theta_1(2\eta|2\tau)}.$$

Applying (A.15), we obtain

$$1 - \zeta^2 + 2\Gamma = \frac{\theta_4(0|2\tau)^3\theta_1(3\eta|\tau)\theta_2(\eta|\tau)}{\theta_1(2\eta|2\tau)\theta_4(2\eta|2\tau)^4}.$$

Using (A.5) and (A.6), this can be written in the desired form. □

Lemma A.2. *The identity* (3.14) *holds.*

Proof. We differentiate (A.19) with respect to η. Setting $\eta = \pi/3$ and applying (A.11) leads to

$$\zeta\zeta_\eta - \Gamma_\eta\big|_{\eta=\pi/3} = \frac{3}{2}\frac{\theta_1'(0|\tau)\theta_3(0|\tau)^4\theta_4(0|\tau)^4}{\theta_1(\pi/3|\tau)\theta_3(\pi/3|\tau)^4\theta_4(\pi/3|\tau)^4} = 24\frac{\theta_1'(0|\tau)\theta_2(\pi/3|\tau)^4}{\theta_1(\pi/3|\tau)\theta_2(0|\tau)^4}. \tag{A.20}$$

Moreover, we evaluate the ratio b_u/a at $u = \eta = \pi/3$ by differentiating (3.2) with respect to the spectral parameter u. Applying (A.5), (A.6) and (A.11) yields

$$\begin{aligned}
\frac{b_u}{a}\bigg|_{u=\eta=\pi/3} &= \frac{\theta_1'(0|2\tau)\theta_4(2\pi/3|2\tau)}{\theta_4(0|2\tau)\theta_1(2\pi/3|2\tau)} = \frac{\theta_1'(0|\tau)\theta_2(0|\tau)\theta_3(\pi/3|\tau)\theta_4(\pi/3|\tau)}{2\,\theta_3(0|\tau)\theta_4(0|\tau)\theta_1(\pi/3|\tau)\theta_2(\pi/3|\tau)} \\
&= \frac{\theta_1'(0|\tau)\theta_2(0|\tau)^2}{4\,\theta_1(\pi/3|\tau)\theta_2(\pi/3|\tau)^2}.
\end{aligned}$$

Combining these two expression gives the desired result. □

Lemma A.3. *In the notation introduced in the main text,*

$$2n\left(\frac{\phi''}{\phi} - \left(\frac{\phi'}{\phi}\right)^2\right)\bigg|_{u=\pi/3} + (2n+1)E = -(2n+1)\frac{\chi(\gamma^2-3)}{(\gamma+1)^2}.$$

Proof. Recall that $\phi = \theta_1^{2n+1}$, where $\theta_1 = \theta_1(u|\tau)$. Hence,

$$\frac{\phi''}{\phi} - \left(\frac{\phi'}{\phi}\right)^2 = (\log\theta_1^{2n+1})'' = (2n+1)\left(\frac{\theta_1''}{\theta_1} - \left(\frac{\theta_1'}{\theta_1}\right)^2\right).$$

It is clear from (3.38) that

$$E = 2nF + G,$$

where

$$\frac{\theta_1(u|\tau)}{\theta_1(3u|3\tau)} = F_0 + F_0 F u^2 + \mathcal{O}(u^4),$$

$$\frac{\theta_1(u|\tau)^3}{\theta_4(3u|3\tau)} = G_0 u^3 + G_0 G u^5 + \mathcal{O}(u^7).$$

Thus, it is enough to show that

$$F = -\frac{\theta_1''}{\theta_1} + \left(\frac{\theta_1'}{\theta_1}\right)^2 \Bigg|_{u=\frac{\pi}{3}}, \tag{A.21}$$

$$G = -\chi \frac{\gamma^2 - 3}{(\gamma + 1)^2} = \chi \frac{\zeta^2 - 6\zeta - 3}{2(\zeta + 1)^2}. \tag{A.22}$$

By (A.10),

$$\frac{\theta_1(u|\tau)}{\theta_1(3u|3\tau)} = \frac{C}{\theta_1\left(\frac{\pi}{3} + u|\tau\right)\theta_1\left(\frac{\pi}{3} - u|\tau\right)},$$

where C is independent of u. On the other hand, by direct Taylor expansion,

$$\frac{\theta_1\left(\frac{\pi}{3} + u|\tau\right)\theta_1\left(\frac{\pi}{3} - u|\tau\right)}{\theta_1\left(\frac{\pi}{3}|\tau\right)^2} = 1 + \left(\frac{\theta_1''}{\theta_1} - \left(\frac{\theta_1'}{\theta_1}\right)^2\right)\Bigg|_{u=\frac{\pi}{3}} u^2 + \mathcal{O}(u^4).$$

This proves (A.21).

To prove (A.22), we consider the function

$$f(u) = \frac{\theta_4\left(\frac{\pi}{3} + u|\tau\right)\theta_4\left(\frac{\pi}{3} - u|\tau\right)}{\theta_2(u|\tau)\theta_3(u|\tau)}.$$

On the one hand, it follows from (A.9) and (A.10) that

$$f(u) = C\frac{\theta_4(3u|3\tau)\theta_1(u|\tau)}{\theta_1(2u|\tau)},$$

with C independent of u. This implies

$$\frac{f''(0)}{2f(0)} = -G. \tag{A.23}$$

On the other hand, it follows from (A.14) that

$$f(u) = \frac{1}{\theta_4(0|\tau)^2}\left(\theta_3\left(\frac{\pi}{3}\Big|\tau\right)^2 \frac{\theta_3(u|\tau)}{\theta_2(u|\tau)} - \theta_2\left(\frac{\pi}{3}\Big|\tau\right)^2 \frac{\theta_2(u|\tau)}{\theta_3(u|\tau)}\right).$$

Differentiating this identity using (A.16) gives

$$f'(u) = \left(\frac{\theta_3(\frac{\pi}{3}|\tau)^2}{\theta_2(u|\tau)^2} + \frac{\theta_2(\frac{\pi}{3}|\tau)^2}{\theta_3(u|\tau)^2}\right)\theta_1(u|\tau)\theta_4(u|\tau)$$

and hence

$$f''(0) = \left(\frac{\theta_3(\frac{\pi}{3}|\tau)^2}{\theta_2(0|\tau)^2} + \frac{\theta_2(\frac{\pi}{3}|\tau)^2}{\theta_3(0|\tau)^2} \right) \theta_1'(0|\tau)\theta_4(0|\tau).$$

Using also (A.4), it follows that

$$\frac{f''(0)}{f(0)} = \frac{\theta_1'(0|\tau)^2}{2\theta_4(\pi/3|\tau)^2} \left(\frac{\theta_3(\pi/3|\tau)^2}{\theta_2(0|\tau)^2} + \frac{\theta_2(\pi/3|\tau)^2}{\theta_3(0|\tau)^2} \right). \tag{A.24}$$

We now use (A.17) to write

$$\frac{\theta_3(\pi/3|\tau)^2}{\theta_2(0|\tau)^2} = \frac{\theta_2(\pi/3|\tau)^2\theta_4(\pi/3|\tau)^2}{\theta_1(\pi/3|\tau)^2\theta_2(0|\tau)^2} \frac{3-\zeta}{1+\zeta},$$

$$\frac{\theta_2(\pi/3|\tau)^2}{\theta_3(0|\tau)^2} = \frac{\theta_2(\pi/3|\tau)^2\theta_4(\pi/3|\tau)^2}{\theta_1(\pi/3|\tau)^2\theta_2(0|\tau)^2} \frac{4\zeta}{(1+\zeta)^2}.$$

Inserting these expressions in (A.24) and comparing with (A.23) gives (A.22). $\square$

Lemma A.4. *The identity* (3.48) *holds.*

Proof. Since $\gamma + 1 = 2(\zeta + 1)/(\zeta - 1)$, it follows from (A.7), (A.8) and (A.17) that

$$\frac{(\gamma+1)^2}{\chi} = 4 \left(\frac{\theta_2(0|\tau)\theta_3(0|\tau)\theta_1(\pi/3|\tau)\theta_4(\pi/3|\tau)}{\theta_1'(0|\tau)\theta_4(0|\tau)\theta_2(\pi/3|\tau)\theta_3(\pi/3|\tau)} \right)^2$$

$$= 4 \left(\frac{\theta_2(0|\tau/2)\theta_1(\pi/3|\tau/2)}{\theta_1'(0|\tau/2)\theta_2(\pi/3|\tau/2)} \right)^2.$$

Using (A.10), it is easy to verify that

$$\frac{\theta_1'(0|3\tau/2)}{\theta_2(0|3\tau/2)} = \frac{1}{3} \frac{\theta_1'(0|\tau/2)\theta_1(\pi/3|\tau/2)^2}{\theta_2(0|\tau/2)\theta_2(\pi/3|\tau/2)^2},$$

$$\frac{h(u+\pi+\frac{\pi\tau}{2})}{h(u+\frac{\pi\tau}{2})} = i\frac{\theta_1(\frac{u}{2}|\frac{\tau}{2})}{\theta_2(\frac{u}{2}|\frac{\tau}{2})} \left(\frac{\theta_2(\frac{\pi}{3}+\frac{u}{2}|\frac{\tau}{2})\theta_2(\frac{\pi}{3}-\frac{u}{2}|\frac{\tau}{2})}{\theta_1(\frac{\pi}{3}+\frac{u}{2}|\frac{\tau}{2})\theta_1(\frac{\pi}{3}-\frac{u}{2}|\frac{\tau}{2})} \right)^n,$$

$$\frac{k(u)}{k(u+\pi)} = \left(\frac{\theta_2(\frac{\pi}{3}+\frac{u}{2}|\frac{\tau}{2})\theta_2(\frac{\pi}{3}-\frac{u}{2}|\frac{\tau}{2})}{\theta_1(\frac{\pi}{3}+\frac{u}{2}|\frac{\tau}{2})\theta_1(\frac{\pi}{3}-\frac{u}{2}|\frac{\tau}{2})} \right)^2 \left(\frac{\theta_4(\frac{\pi}{3}+\frac{u}{2}|\frac{\tau}{2})\theta_4(\frac{\pi}{3}-\frac{u}{2}|\frac{\tau}{2})}{\theta_3(\frac{\pi}{3}+\frac{u}{2}|\frac{\tau}{2})\theta_3(\frac{\pi}{3}-\frac{u}{2}|\frac{\tau}{2})} \right)^{n-2}$$

and hence

$$\frac{h'(\pi+\frac{\pi\tau}{2})}{h(\frac{\pi\tau}{2})} = \frac{i}{2}\frac{\theta_1'(0|\frac{\tau}{2})}{\theta_2(0|\frac{\tau}{2})} \left(\frac{\theta_2(\frac{\pi}{3}|\frac{\tau}{2})}{\theta_1(\frac{\pi}{3}|\frac{\tau}{2})} \right)^{2n},$$

$$\frac{k(0)}{k(\pi)} = \left(\frac{\theta_2(\frac{\pi}{3}|\frac{\tau}{2})}{\theta_1(\frac{\pi}{3}|\frac{\tau}{2})} \right)^4 \left(\frac{\theta_4(\frac{\pi}{3}|\frac{\tau}{2})}{\theta_3(\frac{\pi}{3}|\frac{\tau}{2})} \right)^{2n-4}.$$

Finally, it follows from [40, Lemma 9.1] that

$$2z+1 = -\left(\frac{\theta_1(\frac{\pi}{3}|\frac{\tau}{2})\theta_3(\frac{\pi}{3}|\frac{\tau}{2})}{\theta_2(\frac{\pi}{3}|\frac{\tau}{2})\theta_4(\frac{\pi}{3}|\frac{\tau}{2})} \right)^2,$$

$$\frac{z+1}{z-1} = \left(\frac{\theta_2(\frac{\pi}{3}|\frac{\tau}{2})\theta_3(\frac{\pi}{3}|\frac{\tau}{2})}{\theta_1(\frac{\pi}{3}|\frac{\tau}{2})\theta_4(\frac{\pi}{3}|\frac{\tau}{2})} \right)^2.$$

Combining all these identities gives the desired result. $\square$

Appendix B. Consistency of Differential Equations

The difference-differential equation (3.29) has a similar structure as the non-stationary Lamé equation for $q(u)$ found by Bazhanov and Mangazeev [7], but with the τ-derivative replaced by a shift in the spectral variable. In this Appendix, we give a direct link between these two equations.

The non-stationary Lamé equation can be written

$$\frac{6\mathrm{i}}{\pi}\psi_\tau = \psi_{uu} - V_0\psi, \tag{B.1}$$

where

$$\psi = C\frac{\theta_1(u|\tau)^{2n+1}q(u|\tau)}{\theta_1(3u|3\tau)^n},$$

$C = C(\tau)$ is an appropriate normalizing factor independent of u and

$$V_0 = n(n+1)\wp(u|\pi/3, \pi\tau).$$

After a change of variables, (B.1) can be identified with a special case of the quantum Painlevé VI equation (1.5).

We also need the function

$$\Psi = \psi^1 \wedge \psi^2 = \psi^1(u)\psi^2(v) - \psi^2(u)\psi^1(v),$$

where $\psi^1(u) = \theta_3(3u/2|3\tau/2)\psi(u)$ and $\psi^2(u) = \psi^1(u+\pi)$. It is related to (3.34) by a prefactor. It follows from [43, Thm. 3.1] that

$$\frac{12\mathrm{i}}{\pi}\Psi_\tau = \Psi_{uu} + \Psi_{vv} - (V_0(u) + V_0(v) - 2A)\Psi, \tag{B.2}$$

for some $A = A(\tau)$ independent of u and v. Equivalently,

$$\left(\frac{12\mathrm{i}}{\pi}\psi_\tau^1 - \psi_{uu}^1 + (V_0 - A)\psi^1\right) \wedge \psi^2$$
$$+\psi^1 \wedge \left(\frac{12\mathrm{i}}{\pi}\psi_\tau^2 - \psi_{uu}^2 + (V_0 - A)\psi^2\right) = 0. \tag{B.3}$$

We claim that in fact each of the two terms in (B.3) vanishes. The vanishing of the first term is equivalent to

$$\frac{12\mathrm{i}}{\pi}\psi_\tau^1 - \psi_{uu}^1 + V_0\psi^1 = A\psi^1 + B\psi^2, \tag{B.4}$$

for some $B = B(\tau)$ independent of u. Replacing u by $u + \pi$ gives the vanishing of the second term.

We now use (B.1) to eliminate the τ-derivative in (B.4). The factor $\vartheta = \theta_3(3u/2|3\tau/2)$ satisfies $6\mathrm{i}\vartheta_\tau = \pi\vartheta_{uu}$. Hence,

$$\frac{6\mathrm{i}}{\pi}\psi_\tau^1 = \vartheta\psi_{uu} + \vartheta_{uu}\psi - V_0\vartheta\psi$$
$$= \psi_{uu}^1 - 2\frac{\vartheta_u}{\vartheta}\psi_u^1 + \left(2\left(\frac{\vartheta_u}{\vartheta}\right)^2 - V_0\right)\psi^1.$$

Substituting this into (B.4) gives

$$\psi_{uu}^1 - 4\frac{\vartheta_u}{\vartheta}\psi_u^1 + \left(4\left(\frac{\vartheta_u}{\vartheta}\right)^2 - V_0\right)\psi^1 = A\psi^1 + B\psi^2.$$

In order to get rid of the ψ_u^1-term, we multiply with ϑ^{-2}. After a straightforward computation, we find that the function $\tilde{\psi} = \psi^1/\vartheta^2 = \psi/\vartheta$ satisfies

$$\tilde{\psi}_{uu} + (2(\log\vartheta)_{uu} - V_0)\tilde{\psi} = A\tilde{\psi} + B\frac{\theta_4(3u/2|3\tau/2)\psi(u+\pi)}{\theta_3(3u/2|3\tau/2)^2}.$$

This is precisely (3.29), where we also need the elliptic function identity

$$(\log\vartheta)_{uu} = -\wp\left(u + \pi + \frac{\pi\tau}{2}\Big|\frac{2\pi}{3}, \pi\tau\right) + D,$$

where D is independent of u. This shows that, given (B.1), the equations (3.29) and (B.4) are equivalent. That is, the difference-differential equation (3.29) is a sufficient condition for the mutual consistency of the two differential equations (B.1) and (B.2).

Appendix C. Special Polynomials

In this appendix, we collect some identities related to the polynomials s_n and $\bar{s}_n$. In [43, §5.2], the second author identified them as a special case of the more general rational functions $t^{(k_0,k_1,k_2,k_3)}$. Replacing ζ by $-z-1$ in the relevant identities gives

$$s_n\left(\gamma^{-2}\right) = \left(\frac{(-1)(z-1)}{2z^2(z+1)^2(2z+1)}\right)^{\frac{n(n-1)}{2}} t^{(n,n,0,0)}(-z-1), \tag{C.1a}$$

$$\bar{s}_n\left(\gamma^{-2}\right) = \frac{(-1)^{\frac{(n+1)(n+2)}{2}}(z-1)^{\frac{(n-1)(n+2)}{2}}}{(2z^2(2z+1))^{\frac{n(n-1)}{2}}(z+1)^{n^2-1}} t^{(n,n,1,-1)}(-z-1), \tag{C.1b}$$

where γ and z are related as in (A.18).
We will need further relations that can be obtained from (C.1) using symmetries of the t-polynomials. First of all, applying [43, Prop. 2.3] gives

$$s_{-n-1}\left(\gamma^{-2}\right) = \frac{(-1)^{\frac{(n-1)(n-2)}{2}}3^n(z-1)^{\frac{n^2-5n+2}{2}}}{2^{\frac{n^2-n+2}{2}}z^{n(n-5)}(z+1)^{(n-1)(n-2)}(z+2)^2(2z+1)^{\frac{n^2-n+2}{2}}}$$
$$\times t^{(n,n,-1,-1)}(-z-1), \tag{C.2a}$$

$$\bar{s}_{-n-1}\left(\gamma^{-2}\right) = \frac{(-1)^{\frac{n(n+1)}{2}}3^n(z-1)^{\frac{n^2-7n+2}{2}}}{2^{\frac{n^2-n+2}{2}}z^{n(n-5)}(z+1)^{n^2-4n+2}(z+2)^2(2z+1)^{\frac{n^2-n+6}{2}}}$$
$$\times t^{(n,n,-2,0)}(-z-1). \tag{C.2b}$$

It follows from [43, Prop. 2.2] that

$$t^{(k_0,k_1,k_2,k_3)}(-z-1) = \left(\frac{(-1)^{k_1+k_3}(z+1)^{k_1+k_2-n}(z+2)^{k_2+k_3}}{z^{k_2+k_3-n}(z-1)^{k_1+k_2}}\right)^{n-1} t^{(k_0,k_3,k_2,k_1)}(z),$$

where $n = (k_0 + k_1 + k_2 + k_3)/2$. Applying this transformation to (C.1) and (C.2a) gives

$$s_n\left(\gamma^{-2}\right) = \left(\frac{(-1)}{2(z+1)^2(z-1)(2z+1)}\right)^{\frac{n(n-1)}{2}} t^{(n,0,0,n)}(z), \tag{C.3a}$$

$$\bar{s}_n\left(\gamma^{-2}\right) = \frac{(-1)^{\frac{n(n+1)}{2}}}{\left(2(z+1)^2(z-1)(2z+1)\right)^{\frac{n(n-1)}{2}}} t^{(n,-1,1,n)}(z), \tag{C.3b}$$

$$s_{-n-1}\left(\gamma^{-2}\right) = \frac{(-1)^{\frac{(n-1)(n-2)}{2}} 3^n z^{4n-2}}{(2(z-1)(2z+1))^{\frac{n^2-n+2}{2}}(z+1)^{(n-1)(n-2)}(z+2)^{2n-2}}$$
$$\times t^{(n,-1,-1,n)}(z). \tag{C.3c}$$

Finally, combining [43, Prop. 2.2] and [43, Prop. 2.4] gives

$$t^{(k_0,k_1,k_2,k_3)}(-z-1)$$
$$= (-1)^{(k_1+k_2+n)(k_1+k_3+n)} \frac{Y_{n-k_0}Y_{n-k_1}Y_{n-k_2}Y_{n-k_3}}{Y_{k_0}Y_{k_1}Y_{k_2}Y_{k_3}}$$
$$\times \left(\frac{z^{k_0+k_1-n}(z+1)^{k_1+k_2-n}(z+2)^{k_2+k_3}}{(z-1)^{k_1+k_2}(2z+1)^{k_1+k_3-n}}\right)^{n-1} t^{(n-k_2,n-k_1,n-k_0,n-k_3)}(z),$$

where again $n = (k_0 + k_1 + k_2 + k_3)/2$ and Y_k are elementary coefficients satisfying

$$Y_{k+1}Y_{k-1} = 2(2k+1)Y_k^2, \qquad Y_0 = Y_1 = 1.$$

Applying this to (C.2b) gives

$$\bar{s}_{-n-1}\left(\gamma^{-2}\right) = \frac{(-1)^{\frac{n(n+1)}{2}} 3^n(2n+1)z^{4n-2}}{2^{\frac{n^2-n+2}{2}}(z+1)^{n(n-3)}(z-1)^{\frac{n^2-n+6}{2}}(z+2)^{2n-2}(2z+1)^{\frac{n^2+n+2}{2}}}$$
$$\times t^{(n+1,-1,-1,n-1)}(z). \tag{C.3d}$$

Appendix D. Infinite-Lattice Limit

Correlation functions for the infinite-length XYZ spin chain have been studied by various methods, see e.g. [4,11,26,27,35,44]. In this appendix, we will sketch how such correlation functions can be computed in the special case of interest to us. We have not made a detailed comparison with more general results available in the literature, but the remark at the end of [11, §4.1] indicates that our expression should agree with [11, Eq. (4.2)], after a suitable identification of parameters.

In this appendix, we write the lowest eigenvalue of the Hamiltonian for a chain of length L as $L\varepsilon_L$ and use ε for the infinite-lattice limit $\varepsilon = \lim_{L\to\infty}\varepsilon_L$ (assuming convergence). We have shown that when $L = 2n + 1$, our correlations can be expressed in terms of the quantity (3.11),

$$f_n = \left.\frac{\varepsilon_L(2(\varepsilon_L)_\eta + \Gamma_\eta)}{\zeta\zeta_\eta - \Gamma_\eta}\right|_{\eta=\pi/3}.$$

If we let $n \to \infty$, we find that identical expressions (2.5) hold for the correlations, but with f_n replaced by

$$f_\infty = \lim_{n \to \infty} f_n = \left. \frac{\varepsilon(2\varepsilon_\eta + \Gamma_\eta)}{\zeta \zeta_\eta - \Gamma_\eta} \right|_{\eta = \pi/3}. \tag{D.1}$$

We will compute f_∞ directly using Baxter's explicit expression for ε. We note that Baxter obtained this expression, and several of its properties, by considering the infinite-lattice limit along chains of even length. In contrast, we focus on odd lengths. Hence, we need to assume that the limits along chains of even and odd lengths lead to the same result. Although this assumption seems plausible, we have no proof that it holds.
We start from [5, (10.14.30)], written in Baxter's notation as

$$\varepsilon = \frac{-J_x + J_y + J_z}{2}$$
$$- \frac{\pi (J_x^2 - J_y^2)^{1/2}}{2I\sqrt{k}} \sum_{m=1}^{\infty} \frac{x^{-m}(x^{3m} - q^{m/2})(1 - q^{m/2}x^{-m})(1 - x^{2m})}{(1 - q^m)(1 + x^{2m})}. \tag{D.2}$$

Here, I, k, q, x are functions of the spin chain's anisotropy parameters. The expression for ε holds in the so-called principal regime, defined through the inequalities

$$|J_y| < J_x < -J_z.$$

The values in other regimes follow from the fact that ε is invariant if the parameters (J_x, J_y, J_z) are permuted or if any two of them are multiplied by -1.
We parametrize the chain as in (3.5), (3.7), where we now take $\eta \in \mathbb{R}$ and $\tau \in i\mathbb{R}_{>0}$. One can show that $0 < \zeta < 1$ and hence $|J_z| < J_y < J_x$. Thus, we should apply (D.2) with the replacements $(J_x, J_y, J_z) \mapsto (J_y, -J_z, -J_x)$. The parameters in (D.2) are related to ours by

$$q^{1/2} = e^{-\pi i/\tau}, \qquad x = e^{i(2\eta - \pi)/\tau}$$

and one can compute

$$\frac{\pi}{2I\sqrt{k}} = \frac{2i}{\tau \theta_4(0|\tau)^2}, \qquad (J_y^2 - J_z^2)^{1/2} = \frac{2\theta_4(0|\tau)^2 \theta_1(2\eta|2\tau)}{\theta_2(0|\tau)^2 \theta_4(2\eta|2\tau)}.$$

These replacements lead us to the identity

$$\varepsilon = -\frac{J_x + J_y + J_z}{2}$$
$$- \frac{4i\theta_1(2\eta|2\tau)}{\tau \theta_2(0|\tau)^2 \theta_4(2\eta|2\tau)} \sum_{m=1}^{\infty} \frac{x^{-m}(x^{3m} - q^{m/2})(1 - q^{m/2}x^{-m})(1 - x^{2m})}{(1 - q^m)(1 + x^{2m})}. \tag{D.3}$$

The supersymmetric case $\eta = \pi/3$ corresponds to $x^3 = q^{1/2}$. In this case, all terms in the infinite series vanish and we recover (1.2), that is,

$$\left. \varepsilon \right|_{\eta = \pi/3} = -\frac{J_x + J_y + J_z}{2} = -\frac{\zeta^2 + 3}{4}. \tag{D.4}$$

Let us now consider the quantity $\left. 2\varepsilon_\eta + \Gamma_\eta \right|_{\eta = \pi/3}$. Since $\Gamma = J_x + J_y + J_z - 2$, the contribution from the first term on the right-hand side of (D.3) vanishes. In the remaining

terms, the derivative with respect to η must hit the factor $x^{3m} - q^{m/2}$ to yield a non-zero contribution when $\eta = \pi/3$. It follows that

$$2\varepsilon_\eta + \Gamma_\eta\Big|_{\eta=\pi/3} = \frac{48\,\theta_1(2\pi/3|2\tau)}{\tau^2\theta_2(0|\tau)^2\theta_4(2\pi/3|2\tau)}\,S, \tag{D.5}$$

where

$$S = \sum_{m=1}^\infty \frac{mq^{\frac{m}{3}}(1-q^{\frac{m}{3}})^2}{(1-q^m)(1+q^{\frac{m}{3}})}.$$

To compute S we will use the identity [51, §21, Ex. 11]

$$\frac{\partial}{\partial u}\log\theta_4(u|\tau) = 4\sum_{m=1}^\infty \frac{e^{i\pi\tau m}\sin(2mu)}{1-e^{2i\pi\tau m}}, \qquad |\operatorname{Im}(u)| < \frac{\pi}{2}\operatorname{Im}(\tau),$$

which implies

$$\frac{\partial^2}{\partial u^2}\log\theta_4(u|\tau) = 8\sum_{m=1}^\infty \frac{me^{i\pi\tau m}\cos(2mu)}{1-e^{2i\pi\tau m}}.$$

Rewriting (D.5) with the help of the identity

$$\frac{q^{\frac{m}{3}}(1-q^{\frac{m}{3}})^2}{(1-q^m)(1+q^{\frac{m}{3}})} = q^m\frac{4-3(q^{\frac{m}{3}}+q^{-\frac{m}{3}})+(q^{\frac{2m}{3}}+q^{-\frac{2m}{3}})}{1-q^{2m}}$$

$$= e^{-2\pi im/\tau}\frac{4-6\cos\left(\frac{2\pi m}{3\tau}\right)+2\cos\left(\frac{4\pi m}{3\tau}\right)}{1-e^{-4\pi im/\tau}},$$

it follows that

$$S = \frac{1}{4}\frac{\partial^2}{\partial u^2}\log\frac{\theta_4\left(u|-\frac{2}{\tau}\right)^2\theta_4\left(u+\frac{2\pi}{3\tau}|-\frac{2}{\tau}\right)}{\theta_4\left(u+\frac{\pi}{3\tau}|-\frac{2}{\tau}\right)^3}\Bigg|_{u=0}.$$

Applying (A.3) gives

$$S = \frac{\tau^2}{16}\frac{\partial^2}{\partial u^2}\log g(u)\Bigg|_{u=0},$$

where

$$g(u) = \frac{\theta_2\left(u|\frac{\tau}{2}\right)^2\theta_2\left(u+\frac{\pi}{3}|\frac{\tau}{2}\right)}{\theta_2\left(u+\frac{\pi}{6}|\frac{\tau}{2}\right)^3}.$$

Inserting this expression in (D.5), we obtain

$$2\varepsilon_\eta + \Gamma_\eta\Big|_{\eta=\pi/3} = \frac{3\theta_1(2\pi/3|2\tau)}{\theta_2(0|\tau)^2\theta_4(2\pi/3|2\tau)}\frac{\partial^2}{\partial u^2}\log g(u)\Bigg|_{u=0}. \tag{D.6}$$

To proceed, we use some theta function identities. On the one hand, we have

$$\frac{\partial^2}{\partial u^2} \log g(u)\Big|_{u=0} = \frac{g''(0)g(0) - g'(0)^2}{g(0)^2} = \frac{1}{2g(0)^2} \frac{\partial^2}{\partial u^2} g(u)g(-u)\Big|_{u=0}.$$

On the other hand, using (A.12), one can write

$$g(u)g(-u) = \frac{\theta_1(\pi/3|\tau/2)^2}{\theta_2(\pi/3|\tau/2)^2} h(u)^2 - \frac{\theta_2(0|\tau/2)}{\theta_2(\pi/3|\tau/2)} h(u)^3,$$

where

$$h(u) = \frac{\theta_2\left(u|\frac{\tau}{2}\right)^2}{\theta_1\left(\frac{\pi}{3} + u|\frac{\tau}{2}\right)\theta_1\left(\frac{\pi}{3} - u|\frac{\tau}{2}\right)}.$$

Since h is even, it follows that

$$\frac{\partial^2}{\partial u^2} \log g(u)\Big|_{u=0} = \frac{h(0)h''(0)}{2g(0)^2}\left(2\frac{\theta_1(\pi/3|\tau/2)^2}{\theta_2(\pi/3|\tau/2)^2} - 3\frac{\theta_2(0|\tau/2)}{\theta_2(\pi/3|\tau/2)} h(0)\right). \quad (D.7)$$

Again by (A.12),

$$h(u) - h(0) = \frac{\theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2 \theta_1\left(u|\frac{\tau}{2}\right)^2}{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2 \theta_1\left(\frac{\pi}{3} + u|\frac{\tau}{2}\right)\theta_1\left(\frac{\pi}{3} - u|\frac{\tau}{2}\right)},$$

which implies

$$h''(0) = \frac{2\theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2 \theta_1'(0|\frac{\tau}{2})^2}{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^4}.$$

Inserting also

$$g(0) = \frac{\theta_2\left(0|\frac{\tau}{2}\right)^2 \theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)}{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^3}, \qquad h(0) = \frac{\theta_2\left(0|\frac{\tau}{2}\right)^2}{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2}$$

in (D.7) gives

$$\frac{\partial^2}{\partial u^2} \log g(u)\Big|_{u=0} = \frac{\theta_1'(0|\frac{\tau}{2})^2}{\theta_2(0|\frac{\tau}{2})^2}\left(2\frac{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2}{\theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2} - 3\frac{\theta_2(0|\frac{\tau}{2})^3}{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2 \theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)}\right).$$

Using first (A.7)–(A.8) and then (A.17), one checks that

$$2\frac{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2}{\theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2} - 3\frac{\theta_2(0|\frac{\tau}{2})^3}{\theta_1\left(\frac{\pi}{3}|\frac{\tau}{2}\right)^2 \theta_2\left(\frac{\pi}{3}|\frac{\tau}{2}\right)} = 2\frac{3 + \zeta}{1 - \zeta} - 24\frac{1 + \zeta}{(3 + \zeta)(1 - \zeta)}$$

$$= \frac{2(\zeta^2 - 6\zeta - 3)}{(1 - \zeta)(3 + \zeta)}.$$

We insert this expression in (D.6) and arrive at

$$2\varepsilon_\eta + \Gamma_\eta\Big|_{\eta=\pi/3} = 6\frac{\theta_1(2\pi/3|2\tau)}{\theta_2(0|\tau)^2\theta_4(2\pi/3|2\tau)}\frac{\theta_1'(0|\frac{\tau}{2})^2}{\theta_2(0|\frac{\tau}{2})^2}\frac{(\zeta^2 - 6\zeta - 3)}{(1-\zeta)(3+\zeta)}. \tag{D.8}$$

Returning to (D.1), we insert (A.20), (D.4) and (D.8) to obtain

$$f_\infty = -\frac{1}{8}\frac{\theta_1(2\pi/3|2\tau)\theta_1(\pi/3|\tau)\theta_2(0|\tau)^2\theta_1'(0|\tau/2)^2}{\theta_4(2\pi/3|2\tau)\theta_1'(0|\tau)\theta_2(\pi/3|\tau)^4\theta_2(0|\tau/2)^2}\frac{(\zeta^2+3)(\zeta^2-6\zeta-3)}{(1-\zeta)(3+\zeta)}.$$

Using (A.5)–(A.8), we rewrite this expression in terms of theta functions with nome τ. Simplifying the resulting expression with the help of (A.4) and (A.11) gives

$$f_\infty = -\frac{1}{4}\frac{\theta_1(\pi/3|\tau)^2\theta_4(0|\tau)^2}{\theta_2(\pi/3|\tau)^2\theta_3(0|\tau)^2}\frac{(\zeta^2+3)(\zeta^2-6\zeta-3)}{(1-\zeta)(3+\zeta)}.$$

We can then apply (A.17) and finally obtain

$$f_\infty = -\frac{(\zeta^2+3)(\zeta^2-6\zeta-3)}{8(\zeta+1)^2} = \frac{(\gamma^2+3)(\gamma^2-3)}{(\gamma^2-1)^2}, \tag{D.9}$$

where $\gamma = (\zeta+3)/(\zeta-1)$.

We have assumed above that $0 < \zeta < 1$. The expression (D.9) also holds for $\zeta = 0$ by Stroganov's results [45,46], and for $\zeta = 1$, thanks to the triviality of the correlation functions at this point. The value in other regimes follows since f_∞ is invariant under permutations of the anisotropy parameters, that is, it satisfies the same symmetries (2.9) as f_n. This gives the final result (2.12). We repeat that, in the parametrization (2.6), the nearest-neighbour correlation functions for the infinite chain are given by (2.7) with f_n replaced by f_∞. For instance,

$$C^z = 1 - \frac{4f_\infty}{\zeta^2+3} = \begin{cases} \dfrac{\zeta^4 - 6\zeta^2 + 13}{(\zeta^2-1)^2}, & |\zeta| \geq 3, \\[2mm] \dfrac{(\zeta+1)(3\zeta-1)}{2(\zeta-1)^2}, & -3 \leq \zeta \leq 0, \\[2mm] \dfrac{(\zeta-1)(3\zeta+1)}{2(\zeta+1)^2}, & 0 \leq \zeta \leq 3. \end{cases}$$

One can check that the correlation functions are twice differentiable in ζ, but their third derivatives jump at the XXZ points $\zeta = 0$ and $\zeta = \pm 3$.

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