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Topics in Bethe ansatz

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Integrable quantum spin chains have close connections to integrable quantum field theories, modern condensed matter physics, string and Yang-Mills theories. Bethe ansatz is one of the most important approaches for solving quantum integrable spin chains. At the heart of the algebraic structure of integrable quantum spin chains is the quantum Yang-Baxter equation and the boundary Yang-Baxter equation. This thesis focuses on four topics in Bethe ansatz.

The Bethe equations for the isotropic periodic spin-1/2 Heisenberg chain with N sites have solutions containing $\pm i/2$ that are singular: both the corresponding energy and the algebraic Bethe ansatz vector are divergent. Such solutions must be carefully regularized. We consider a regularization involving a parameter that can be determined using a generalization of the Bethe equations. These generalized Bethe equations provide a practical way of determining which singular solutions correspond to eigenvectors of the model.

The Bethe equations for the periodic XXX and XXZ spin chains admit singular solutions, for which the corresponding eigenvalues and eigenvectors are ill-defined. We use a twist regularization to derive conditions for such singular solutions to be

physical, in which case they correspond to genuine eigenvalues and eigenvectors of the Hamiltonian.

We analyze the ground state of the open spin-1/2 isotropic quantum spin chain with a non-diagonal boundary term using a recently proposed Bethe ansatz solution. As the coefficient of the non-diagonal boundary term tends to zero, the Bethe roots split evenly into two sets: those that remain finite, and those that become infinite. We argue that the former satisfy conventional Bethe equations, while the latter satisfy a generalization of the Richardson-Gaudin equations. We derive an expression for the leading correction to the boundary energy in terms of the boundary parameters.

We argue that the Hamiltonians for $A_{2n}^{(2)}$ open quantum spin chains corresponding to two choices of integrable boundary conditions have the symmetries $U_q(B_n)$ and $U_q(C_n)$, respectively. The deformation of C_n is novel, with a nonstandard coproduct. We find a formula for the Dynkin labels of the Bethe states (which determine the degeneracies of the corresponding eigenvalues) in terms of the numbers of Bethe roots of each type. With the help of this formula, we verify numerically (for a generic value of the anisotropy parameter) that the degeneracies and multiplicities of the spectra implied by the quantum group symmetries are completely described by the Bethe ansatz.

To my parents Zhihou and Guimei

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CHAPTER 1

Introduction

Integrable quantum spin chains have close connections to integrable quantum field theories [1–4], modern condensed matter physics [5, 6], string and Yang-Mills theories [7,8]. At the heart of the algebraic structure of integrable quantum spin chains is the quantum Yang-Baxter equation (YBE) [9] and the boundary Yang-Baxter equation (BYBE) [3, 10, 11]. Closed integrable spin chains can be constructed using only solutions of the YBE, while open integrable spin chains are constructed with solutions of the BYBE, in addition to YBE [3, 11, 12].

Bethe ansatz (BA) [13] is one of the most important approaches for solving quantum integrable spin chains. Several methods for deriving BA solutions of quantum integrable models have been developed: the coordinate BA [13–16], the analytical BA [17–19], the algebraic BA [9, 20] and others (see e.g. [21]).

In this thesis we will focus primarily on the algebraic BA, developed by Faddeev's school since the 1980's, originally introduced to solve closed chains [9], and subsequently generalized by Sklyanin to solve open chains [11]. We will consider four problems related to Bethe ansatz for both closed and open chains. In the next two sections of this chapter, we will briefly review the construction and procedure of using Bethe ansatz to solve the XXX spin-$\frac{1}{2}$ periodic chain and the XXX spin-$\frac{1}{2}$ open chain. In the last section of this chapter we introduce the four problems that are the subject of this thesis.

1.1 Closed chains

We begin by reviewing the general construction of integrable closed chains with periodic boundary conditions. We then focus on the isotropic (XXX) periodic spin-$\frac{1}{2}$ quantum chain with N sites, which has the following Hamiltonian:

$$H = \frac{1}{4}\sum_{n=1}^{N} \left(\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - I\right) \,, \qquad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1 \,, \tag{1.1}$$

where I is identity matrix. Direct diagonalization of this Hamiltonian, which is a $2^N \times 2^N$ matrix, is not practical for large N. A useful alternative is (algebraic) Bethe ansatz, which we also review [9, 20].

1.1.1 Permutation matrix

Let $V = C^n$ be an n-dimensional complex vector space. The permutation matrix on $V \otimes V$ is defined by:

$$P(v \otimes w) = w \otimes v, \text{ where}\, w,\, v \in V. \tag{1.2}$$

For any linear operator X that maps V to V, we have the following relation:

$$P_{12} X_1 P_{12} = X_2 \,. \tag{1.3}$$

1.1.2 R-matrix and Yang-Baxter equation

The R-matrix $R(\lambda)$ is a matrix that maps $V \otimes V$ to $V \otimes V$, and is a function of the complex variable λ, which is called "spectral parameter". Using this matrix, we can construct operators acting on 3 copies of V (i.e. $V \otimes V \otimes V$):

$$
\begin{aligned}
R_{12}(\lambda) &= R(\lambda) \otimes I \\
R_{23}(\lambda) &= I \otimes R(\lambda) \\
R_{13}(\lambda) &= P_{23} R_{12}(\lambda) P_{23}\,,
\end{aligned}
\tag{1.4}
$$

where I is the identity matrix, and $P_{23} = I \otimes P$. By definition, the R-matrix is a solution of the Yang-Baxter equation (YBE):

$$
R_{12}(\lambda_1 - \lambda_2) R_{13}(\lambda_1) R_{23}(\lambda_2) = R_{23}(\lambda_2) R_{13}(\lambda_1) R_{12}(\lambda_1 - \lambda_2)\,. \tag{1.5}
$$

We also assume that the R-matrix has the regularity property

$$
R(0) \propto P\,. \tag{1.6}
$$

1.1.3 Monodromy matrix and transfer matrix

The monodromy matrix is defined as follows

$$
T_a(\lambda) = R_{aN}(\lambda) \cdots R_{a1}(\lambda)\,, \tag{1.7}
$$

where a stands for auxiliary space, which obeys the following so-called RTT relation

$$
R_{aa'}(\lambda_1 - \lambda_2) T_a(\lambda_1) T_{a'}(\lambda_2) = T_{a'}(\lambda_2) T_a(\lambda_1) R_{aa'}(\lambda_1 - \lambda_2)\,, \tag{1.8}
$$

as follows from the YBE. The transfer matrix $t(\lambda)$ is defined by tracing the monodromy matrix $T_a(\lambda)$ over the auxiliary space

$$
t(\lambda) = tr_a T_a(\lambda) \quad , \tag{1.9}
$$

which satisfies

$$[t(\lambda_1), t(\lambda_2)] = 0 \ , \tag{1.10}$$

as follows from the RTT relation. We define the Hamiltonian $H \propto \frac{d}{d\lambda} ln(t(\lambda))|_{\lambda=0}$, which commutes with the transfer matrix

$$[t(\lambda), H] = 0 \ . \tag{1.11}$$

Equations (1.10) and (1.11) imply that the model is integrable.

1.1.4 Algebraic Bethe ansatz

We now consider the XXX spin-$\frac{1}{2}$ chain. For this model, $V = C^2$, and the R-matrix, satisfying the YBE (1.5), is given by the 4×4 matrix

$$R(\lambda) = \lambda I + iP \ , \tag{1.12}$$

where I is identity matrix, and the permutation matrix P is given by

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \tag{1.13}$$

One can show that the Hamiltonian (1.1) is related to the transfer matrix (1.9) by

$$H = \frac{1}{2}(i\frac{d}{d\lambda} ln(t(\lambda))|_{\lambda=0} - NI^{\otimes N}) \tag{1.14}$$

The monodromy matrix $T_a(\lambda)$ (1.7) can be expressed as a 2×2 matrix in the auxiliary space whose matrix elements $A(\lambda)$, $B(\lambda)$, $C(\lambda)$ and $D(\lambda)$ are operators acting on the quantum space $V^{\otimes N}$,

$$T_a(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} . \tag{1.15}$$

A set of algebraic relations among these four operators can be extracted from the RTT relation (1.8). We list the relations necessary for our purpose below

$$\begin{aligned} [B(\lambda_1), B(\lambda_2)] &= 0 \\ A(\lambda_1)B(\lambda_2) &= \frac{a(\lambda_2-\lambda_1)}{b(\lambda_2-\lambda_1)} B(\lambda_2)A(\lambda_1) - \frac{c(\lambda_2-\lambda_1)}{b(\lambda_2-\lambda_1)} B(\lambda_1)A(\lambda_2) \\ D(\lambda_1)B(\lambda_2) &= \frac{a(\lambda_1-\lambda_2)}{b(\lambda_1-\lambda_2)} B(\lambda_2)D(\lambda_1) - \frac{c(\lambda_1-\lambda_2)}{b(\lambda_1-\lambda_2)} B(\lambda_1)D(\lambda_2)\,, \end{aligned} \tag{1.16}$$

where $a(\lambda) = \lambda + i$, $b(\lambda) = \lambda$, $c(\lambda) = i$. Define ω_+ as the reference state with all spins up

$$\omega_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}^{\otimes N} , \tag{1.17}$$

which is an eigenvector of $A(\lambda)$ and $D(\lambda)$

$$A(\lambda)\omega_+ = (\lambda + i)^N \omega_+, \qquad D(\lambda)\omega_+ = \lambda^N \omega_+, \qquad C(\lambda)\omega_+ = 0\,. \tag{1.18}$$

We use $B(\lambda)$ as a creation operator acting on ω_+ to get the so-called Bethe vector

$$|\lambda_1, \cdots, \lambda_m\rangle = B(\lambda_1) \cdots B(\lambda_m)\omega_+\,. \tag{1.19}$$

Applying the transfer matrix $t(\lambda) = A(\lambda) + D(\lambda)$ to $|\lambda_1, \cdots, \lambda_m\rangle$ and moving $A(\lambda)$ and $D(\lambda)$ through the B's with the help of the exchange relations (1.16), one can show [9] that $|\lambda_1, \cdots, \lambda_m\rangle$ is an eigenvector of $t(\lambda)$

$$t(\lambda)|\lambda_1, \cdots, \lambda_m\rangle = \Lambda(\lambda)|\lambda_1, \cdots, \lambda_m\rangle\,, \tag{1.20}$$

with eigenvalue $\Lambda(\lambda)$ given by

$$\Lambda(\lambda) = (\lambda + i)^N \prod_{j=1}^{m} \left(\frac{\lambda - \lambda_j - i}{\lambda - \lambda_j} \right) + \lambda^N \prod_{j=1}^{m} \left(\frac{\lambda - \lambda_j + i}{\lambda - \lambda_j} \right) , \tag{1.21}$$

if $\lambda_1, \cdots, \lambda_m$ are distinct and satisfy the Bethe ansatz equations (BAE)

$$\left(\frac{\lambda_j + i}{\lambda_j} \right)^N = \prod_{k \neq j}^{m} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}, \qquad j = 1, \cdots, m \, . \tag{1.22}$$

The corresponding energy of the Hamiltonian can be expressed in terms of the solutions of the BAEs (1.22) as follows

$$E = -\frac{1}{2} \sum_{k=1}^{m} \frac{1}{\lambda_k(\lambda_k + i)} \, . \tag{1.23}$$

The eigenvalue expression (1.20) can be rewritten as the so-called $T - Q$ equation

$$Q(\lambda)\Lambda(\lambda) = (\lambda + i)^N Q(\lambda - i) + \lambda^N Q(\lambda + i) \tag{1.24}$$

with

$$Q(\lambda) = \prod_{k=1}^{m} (\lambda - \lambda_k) \tag{1.25}$$

1.2 Open chains

We turn now to the construction and solution of integrable open chains.

1.2.1 Boundary Yang-Baxter equation

We require that the R-matrix satisfy the crossing condition [22, 23]

$$R_{12}(\lambda) = V_1 R_{12}^{t_2}(-\lambda - \rho) V_1 \, . \tag{1.26}$$

With the crossing matrix V solved from the above equation, the matrix M is defined as follows

$$M = V^t V\,. \tag{1.27}$$

Two boundary K-matrices $K^-(\lambda)$ and $K^+(\lambda)$ corresponding to boundary conditions of open chains are the solutions of the corresponding boundary Yang-Baxter equations (BYBE) [3, 10, 11, 22, 23]. For $K^-(\lambda)$ we have

$$R_{12}(\lambda_1-\lambda_2)K_1^-(\lambda_1)R_{21}(\lambda_1+\lambda_2)K_2^-(\lambda_2) = \tag{1.28}$$

$$K_2^-(\lambda_2)R_{12}(\lambda_1+\lambda_2)K_1^-(\lambda_1)R_{21}(\lambda_1-\lambda_2)\,, \tag{1.29}$$

where $R_{21}(\lambda) = P_{12}R_{12}(\lambda)P_{12}$. Similarly, for $K^+(\lambda)$, we have

$$R_{12}(-\lambda_1+\lambda_2)K_1^{+t_1}(\lambda_1)M_1^{-1}R_{21}(-\lambda_1-\lambda_2-2\rho)M_1K_2^{+t_2}(\lambda_2) = \tag{1.30}$$

$$K_2^{+t_2}(\lambda_2)M_1R_{12}(-\lambda_1-\lambda_2-2\rho)M_1^{-1}K_1^{+t_1}(\lambda_1)R_{21}(-\lambda_1+\lambda_2)\,. \tag{1.31}$$

1.2.2 Monodromy matrix and transfer matrix

A solution R of the YBE together with its corresponding solutions K^-, K^+ of the BYBE can be used to construct an integrable open chain. To this end, we define the two monodromy matrices

$$T_a(\lambda) = R_{aN}(\lambda)\cdots R_{a1}(\lambda)\,, \tag{1.32}$$

$$\hat{T}_a(\lambda) = R_{1a}(u)\cdots R_{Na}(u)\,. \tag{1.33}$$

The double-row monodromy matrix is defined by [11]

$$U_a(\lambda) = T_a(\lambda)K_a^-(\lambda)\hat{T}_a(\lambda)\,, \tag{1.34}$$

which obeys the same equation as $K^-(\lambda)$, namely,

$$R_{12}(\lambda_1 - \lambda_2)U_1(\lambda_1)R_{21}(\lambda_1 + \lambda_2)U_2(\lambda_2) = \\ U_2(\lambda_2)R_{12}(\lambda_1 + \lambda_2)U_1(\lambda_1)R_{21}(\lambda_1 - \lambda_2)\,. \tag{1.35}$$

Now we can construct transfer matrix as follows [11]

$$t(\lambda) = tr_a K_a^+(\lambda)U_a(\lambda) = tr_a K_a^+(\lambda)T_a(\lambda)K_a^-(\lambda)\hat{T}_a(\lambda)\,, \tag{1.36}$$

which can be shown to have the important property

$$[t(\lambda_1), t(\lambda_2)] = 0\,. \tag{1.37}$$

The corresponding integrable Hamiltonian is given by

$$H \propto \frac{d}{d\lambda}t(\lambda)\Big|_{\lambda=0}\,. \tag{1.38}$$

1.2.3 ABA approach for XXX spin-$\frac{1}{2}$ chain with diagonal boundary terms

The Hamiltonian for the XXX spin-$\frac{1}{2}$ chain with diagonal boundary terms is

$$H = \sum_{j=1}^{N-1} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + \frac{1}{p}\sigma_N^z + \frac{1}{q}\sigma_1^z\,, \tag{1.39}$$

where p and q are arbitrary real boundary parameters. To be consistent with Chapter 4, instead of (1.12), we now use the following R matrix

$$R(\lambda) = \lambda I + P\,. \tag{1.40}$$

It satisfies the crossing relation (1.26) with

$$\rho = 1\,, \qquad V = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1.41}$$

The two boundary K-matrices corresponding to the Hamiltonian (1.39) are as follows

$$K^-(\lambda) = \begin{pmatrix} p+\lambda & 0 \\ 0 & p-\lambda \end{pmatrix}, \qquad K^+(\lambda) = \begin{pmatrix} q+\lambda+1 & 0 \\ 0 & q-\lambda-1 \end{pmatrix}. \tag{1.42}$$

The double-row monodromy matrix (1.34) can be expressed as a 2×2 matrix in the auxiliary space whose matrix elements $\mathcal{A}(\lambda)$, $\mathcal{B}(\lambda)$, $\mathcal{C}(\lambda)$ and $\mathcal{D}(\lambda)$ are operators acting on the quantum space $V^{\otimes N}$,

$$U_a(\lambda) = \begin{pmatrix} \mathcal{A}(\lambda) & \mathcal{B}(\lambda) \\ \mathcal{C}(\lambda) & \mathcal{D}(\lambda) + \frac{1}{2\lambda+1}\mathcal{A}(\lambda) \end{pmatrix}. \tag{1.43}$$

The transfer matrix (1.36) is now given by

$$t(\lambda) = \frac{2(\lambda+q)(\lambda+1)}{2\lambda+1}\mathcal{A}(\lambda) + (q-\lambda-1)\mathcal{D}(\lambda)\,. \tag{1.44}$$

The reference state ω_+ is an eigenvector of $\mathcal{A}(\lambda)$, $\mathcal{C}(\lambda)$ and $\mathcal{D}(\lambda)$,

$$\mathcal{A}(\lambda)\omega_+ = \Lambda_1(\lambda)\omega_+, \qquad \mathcal{D}(\lambda)\omega_+ = \Lambda_2(\lambda)\omega_+, \qquad \mathcal{C}(\lambda)\omega_+ = 0\,, \tag{1.45}$$

where $\Lambda_1(\lambda) = (\lambda+p)(\lambda+1)^{2N}$, $\Lambda_2(\lambda) = \frac{2\lambda}{2\lambda+1}(p-\lambda-1)\lambda^{2N}$.

Using (1.35), we can obtain exchange relations among $\mathcal{A}(\lambda)$, $\mathcal{B}(\lambda)$, $\mathcal{C}(\lambda)$ and $\mathcal{D}(\lambda)$. We list the necessary ones below, following [24]

$$\begin{aligned} [\mathcal{B}(\lambda_1), \mathcal{B}(\lambda_2)] &= 0, \\ \mathcal{A}(\lambda_1)\mathcal{B}(\lambda_2) &= f(\lambda_1,\lambda_2)\mathcal{B}(\lambda_2)\mathcal{A}(\lambda_1) + g(\lambda_1,\lambda_2)\mathcal{B}(\lambda_1)\mathcal{A}(\lambda_2) + w(\lambda_1,\lambda_2)\mathcal{B}(\lambda_1)\mathcal{D}(\lambda_2), \\ \mathcal{D}(\lambda_1)\mathcal{B}(\lambda_2) &= h(\lambda_1,\lambda_2)\mathcal{B}(\lambda_2)\mathcal{D}(\lambda_1) + k(\lambda_1,\lambda_2)\mathcal{B}(\lambda_1)\mathcal{D}(\lambda_2) + n(\lambda_1,\lambda_2)\mathcal{B}(\lambda_1)\mathcal{A}(\lambda_2), \end{aligned} \tag{1.46}$$

where the coefficients are as follows,

$$\begin{aligned}
f(u,v) &= \frac{(u-v-1)(u+v)}{(u-v)(u+v+1)}, & h(u,v) &= \frac{(u-v+1)(u+v+2)}{(u-v)(u+v+1)},\\
w(u,v) &= \frac{-1}{(u+v+1)}, & g(u,v) &= \frac{2v}{(2v+1)(u-v)},\\
k(u,v) &= \frac{-2(u+1)}{(u-v)(2u+1)}, & n(u,v) &= \frac{4v(u+1)}{(u+v+1)(2v+1)(2u+1)}.
\end{aligned} \tag{1.47}$$

We define Bethe states $|\lambda_1, \cdots, \lambda_m\rangle$ similarly to the periodic case (1.19) as follows

$$|\lambda_1, \cdots, \lambda_m\rangle = \mathcal{B}(\lambda_1) \cdots \mathcal{B}(\lambda_m)\omega_+\,, \tag{1.48}$$

where the reference state ω_+ is again given by (1.17). We again apply $t(\lambda)$ to the Bethe vector $|\lambda_1, \cdots, \lambda_m\rangle$, then carry $\mathcal{A}(\lambda)$ and $\mathcal{D}(\lambda)$ through $\mathcal{B}(\lambda_1)$, ..., $\mathcal{B}(\lambda_m)$. With the aid of exchange relations (1.46), we obtain [11, 24]

$$t(\lambda)|\lambda_1, \cdots, \lambda_m\rangle = \Lambda(\lambda)|\lambda_1, \cdots, \lambda_m\rangle\,, \tag{1.49}$$

with

$$\Lambda(\lambda) = \bar{\alpha}(\lambda)\prod_{j=1}^{m}\frac{(\lambda-\lambda_j-1)(\lambda+\lambda_j)}{(\lambda-\lambda_j)(\lambda+\lambda_j+1)} + \bar{\delta}(\lambda)\prod_{j=1}^{m}\frac{(\lambda-\lambda_j+1)(\lambda+\lambda_j+2)}{(\lambda-\lambda_j)(\lambda+\lambda_j+1)}\,, \tag{1.50}$$

where $\bar{\alpha}(\lambda) = \frac{2\lambda+2}{2\lambda+1}(\lambda+p)(\lambda+q)(\lambda+1)^{2N}$, $\bar{\delta}(\lambda) = \bar{\alpha}(-\lambda-1)$, provided that $\lambda_1, \cdots, \lambda_m$ satisfy the following BAEs

$$\begin{aligned}
&\left(\frac{\lambda_j+1}{\lambda_j}\right)^{2N}\left(\frac{\lambda_j+p}{\lambda_j-p+1}\right)\left(\frac{\lambda_j+q}{\lambda_j-q+1}\right) = \prod_{k\neq j}^{m}\frac{\lambda_j-\lambda_k+1}{\lambda_j-\lambda_k-1}\frac{\lambda_j+\lambda_k+2}{\lambda_j+\lambda_k}\\
&j = 1, \cdots, m\,.
\end{aligned} \tag{1.51}$$

We define the new quantity $Q(\lambda) = \prod_{j=1}^{m}(\lambda-\lambda_j)(\lambda+\lambda_j+1)$, the equation (1.50) can be rewritten in the $T-Q$ form

$$\Lambda(\lambda)Q(\lambda) = \bar{\alpha}(\lambda)Q(\lambda-1) + \bar{\delta}(\lambda)Q(\lambda+1)\,. \tag{1.52}$$

The eigenvalues of the Hamiltonian (1.39) are given as follows

$$E = 2\sum_{j=1}^{m} \frac{1}{\lambda_j(\lambda_j+1)} + N - 1 + \frac{1}{p} + \frac{1}{q}\,. \tag{1.53}$$

1.2.4 XXX spin-$\frac{1}{2}$ chain with a nondiagonal boundary term

Let us now consider the Hamiltonian for the XXX spin-$\frac{1}{2}$ chain with a *nondiagonal* boundary term, as well as diagonal boundary terms,

$$H = \sum_{j=1}^{N-1} \vec{\sigma}_j \cdot \vec{\sigma}_{j+1} + \frac{1}{p}\sigma_N^z + \frac{\xi}{q}\sigma_1^x + \frac{1}{q}\sigma_1^z\,, \tag{1.54}$$

where p, q and ξ are arbitrary real boundary parameters. The two K-matrices corresponding to the above Hamiltonian [3, 12] are as follows

$$K^-(\lambda) = \begin{pmatrix} p+\lambda & 0 \\ 0 & p-\lambda \end{pmatrix}, \qquad K^+(\lambda) = \begin{pmatrix} q+\lambda+1 & (\lambda+1)\xi \\ (\lambda+1)\xi & q-\lambda-1 \end{pmatrix}, \tag{1.55}$$

and the transfer matrix is

$$t(\lambda) = \frac{2(\lambda+q)(\lambda+1)}{2\lambda+1}\mathcal{A}(\lambda) + (\lambda+1)\xi(\mathcal{B}(\lambda)+\mathcal{C}(\lambda)) + (q-\lambda-1)\mathcal{D}(\lambda)\,. \tag{1.56}$$

Due to the presence of $\mathcal{B}(\lambda)$ in $t(\lambda)$, the reference state ω_+ is no longer an eigenstate of the transfer matrix, and therefore the conventional ABA method does not work.

An inhomogeneous $T-Q$ equation has been proposed by Cao, Yang, Shi and Wang [25] to overcome this obstacle. One introduces inhomogeneities in the monodromy matrices

$$\begin{aligned} T_a(\lambda) &= R_{aN}(\lambda-\theta_N)R_{aN-1}(\lambda-\theta_{N-1})\cdots R_{a1}(\lambda-\theta_1) \\ \hat{T}_a(\lambda) &= R_{a1}(\lambda+\theta_1)R_{a2}(\lambda+\theta_2)\cdots R_{aN}(\lambda-\theta_N) \end{aligned} \tag{1.57}$$

where $\theta_j|1, \cdots, N$ are arbitrary complex inhomogeneous parameters. Using the crossing relation of the R-matrix (1.26) and expressions of K-matrices, one can show that the transfer matrix has the following properties

$$\text{Crossing symmetry}: \quad t(-\lambda-1) = t(\lambda), \tag{1.58}$$

$$\text{Initial condition}: \; t(0) = 2p\,q\prod_{j=1}^{N}(1-\theta_j)(1+\theta_j) \times \mathrm{I}, \tag{1.59}$$

$$\text{Asymptotic behavior}: \; t(\lambda) \sim 2\lambda^{2N+2} \times \mathrm{I} + \ldots, \quad \text{for}\, \lambda \to \pm\infty. \tag{1.60}$$

which imply that the corresponding eigenvalue $\Lambda(\lambda)$ has the same properties

$$\text{Crossing symmetry}: \quad \Lambda(-\lambda-1) = \Lambda(\lambda), \tag{1.61}$$

$$\text{Initial condition}: \; \Lambda(0) = 2p\,q\prod_{j=1}^{N}(1-\theta_j)(1+\theta_j), \tag{1.62}$$

$$\text{Asymptotic behavior}: \; \Lambda(\lambda) \sim 2\lambda^{2N+2} + \ldots, \quad \text{for}\, \lambda \to \pm\infty. \tag{1.63}$$

The analyticity of the R-matrix and K-matrices, and the independence on λ of the eigenstates, imply that $\Lambda(\lambda)$ must be a polynomial in λ of degree $2N+2$. In addition, one can show using the fusion procedure [26–29] that

$$\begin{aligned} \Lambda(\theta_j)\Lambda(\theta_j-1) = &\; \frac{2(\theta_j+1)(q^2-(1+\xi^2)\theta_j^2)}{(2\theta_j-1)(2\theta_j+1)}a(\theta_j)d(\theta_j-1) \\ j = 1, \cdots, N. \end{aligned} \tag{1.64}$$

with

$$\begin{aligned} a(\lambda) &= (p+\lambda)\prod_{j=1}^{N}(\lambda-\theta_j+1)(\lambda+\theta_j+1), \\ d(\lambda) &= 2\lambda(p-\lambda-1)\prod_{j=1}^{N}(\lambda-\theta_j)(\lambda+\theta_j). \end{aligned} \tag{1.65}$$

An expression for $\Lambda(\lambda)$ that is consistent with all the above conditions (1.61)-(1.64) has been found in [25]. A simplified T-Q equation has been obtained [30], which in the homogeneous limit (all $\theta_j = 0$) is given by

$$\Lambda(\lambda)\, Q(\lambda) = \bar{a}(\lambda)\, Q(\lambda-1) + \bar{d}(\lambda)\, Q(\lambda+1) + 2(1-\sqrt{1+\xi^2})\,(\lambda(\lambda+1))^{2N+1} \tag{1.66}$$

where

$$\bar{a}(\lambda) = \frac{2\lambda+2}{2\lambda+1}(\lambda+p)(\sqrt{1+\xi^2}\lambda+q)(\lambda+1)^{2N}\,, \qquad \bar{d}(\lambda) = \bar{a}(-\lambda-1)\,, \tag{1.67}$$

and

$$Q(\lambda) = \prod_{j=1}^{N}(\lambda-\lambda_j)(\lambda+\lambda_j+1)\,. \tag{1.68}$$

Note the presence of an extra ("inhomogeneous") term in the $T-Q$ equation (1.66). For the diagonal case $\xi = 0$, the previous result (1.52) is recovered. The zeros $\lambda_1, \ldots, \lambda_N$ of $Q(\lambda)$ satisfy the Bethe equations that follow directly from (1.66):

$$\begin{aligned} & e_1(u_j)^{2N}\, e_{2p-1}(u_j)\, e_{2\tilde{q}-1}(u_j) - \prod_{\substack{k \neq j \\ k=1}}^{N} e_2(u_j-u_k)\, e_2(u_j+u_k) \\ & = i\left(1-\frac{1}{\sqrt{1+\xi^2}}\right)\frac{u_j(u_j+\frac{i}{2})^{2N}}{(u_j-i(p-\frac{1}{2}))(u_j-i(\tilde{q}-\frac{1}{2}))\prod_{\substack{k\neq j \\ k=1}}^{N}(u_j-u_k-i)(u_j+u_k-i)}\,, \\ & \qquad j = 1, 2, \ldots, N\,, \end{aligned} \tag{1.69}$$

where

$$u_j = i\left(\lambda_j + \tfrac{1}{2}\right)\,, \qquad \tilde{q} = \frac{q}{\sqrt{1+\xi^2}}\,, \qquad e_n(u) = \frac{u+\frac{in}{2}}{u-\frac{in}{2}}\,. \tag{1.70}$$

The eigenvalues of the Hamiltonian (1.54) are given by [30]

$$E = -2\sum_{j=1}^{N}\frac{1}{u_j^2+\frac{1}{4}} + N - 1 + \frac{1}{p} + \frac{1}{\tilde{q}}\,. \tag{1.71}$$

1.3 Content of the thesis

The remainder of the thesis consists of four publications, which we now introduce.

Chapter 2: Algebraic Bethe ansatz for singular solutions,

R. I. Nepomechie and C. Wang, J.Phys. A46 (2013) 325002, arXiv:1304.7978 [hep-th].

The BAEs (1.22) for the closed XXX spin-$\frac{1}{2}$ chain can be written in a more symmetric form by making the shift $u_j = \lambda_j + \frac{i}{2}$,

$$\left(\frac{u_j + \frac{i}{2}}{u_j - \frac{i}{2}}\right)^N = \prod_{k \neq j}^{M} \frac{u_j - u_k + i}{u_j - u_k - i}, \quad j = 1, \cdots, M\,. \tag{1.72}$$

The expression (1.23) for the energy becomes

$$E = -\frac{1}{2} \sum_{k=1}^{M} \frac{1}{u_k^2 + \frac{1}{4}}\,. \tag{1.73}$$

For $M = 2, N \geq 4$, $(u_1, u_2) = (\frac{i}{2}, -\frac{i}{2})$ is an exact solution of the above BAEs. We can easily see this from the pole-free form of the BAEs

$$\begin{aligned} (u_1 + \frac{i}{2})^N (u_1 - u_2 - i) &= (u_1 - \frac{i}{2})^N (u_1 - u_2 + i) \\ (u_2 + \frac{i}{2})^N (u_2 - u_1 - i) &= (u_2 - \frac{i}{2})^N (u_2 - u_1 + i)\,. \end{aligned} \tag{1.74}$$

Solutions of the form $(\frac{i}{2}, -\frac{i}{2}, \lambda_3, \cdots \lambda_M)$ (where $\lambda_3, \cdots, \lambda_M \neq \pm\frac{i}{2}$) are called "singular" solutions, while solutions without roots $(\frac{i}{2}, -\frac{i}{2})$ are called "regular" solutions.

Singular solutions suffer from two basic problems:

(i) the energy (1.73) is ill-defined

(ii) the Bethe state (1.19) is also ill -defined

There is a naive regularization

$$u_1^{naive} = \frac{i}{2} + \epsilon, \quad u_2^{naive} = -\frac{i}{2} + \epsilon \tag{1.75}$$

that can regularize the energy (1.73); however, the Bethe state (1.19) obtained in this way is not an eigenstate of the Hamiltonian (1.1).

We classify singular solutions into two types: *physical* singular solutions, which correspond to eigenstates of the Hamiltonian; and *unphysical* singular solutions, which do not correspond to eigenstates of the Hamiltonian.

In Chapter 2, we use the following regularization

$$u_1 = \frac{i}{2} + \epsilon + c\epsilon^N, \quad u_2 = -\frac{i}{2} + \epsilon \tag{1.76}$$

(where the constant c is to be determined) to solve the problems (i) and (ii), and also to obtain a criteria to select the singular solutions that are physical, namely

$$\left[-\prod_{k=3}^{M} \left(\frac{u_k + \frac{i}{2}}{u_k - \frac{i}{2}} \right) \right]^N = 1\,. \tag{1.77}$$

Chapter 3: Twisting singular solutions of Bethe's equations

R. I. Nepomechie and C. Wang, J.Phys. A47 (2014) 505004, arXiv:1409.7382 [hep-th].

The regularization (1.76) is somewhat unphysical and ad hoc. In Chapter 3, we consider an alternative way of regularization, a twist angle β in the boundary conditions,

$$\begin{aligned}\sigma^x_{N+1} &= \cos\beta\,\sigma^x_1 - \sin\beta\,\sigma^y_1\,,\\ \sigma^y_{N+1} &= \sin\beta\,\sigma^x_1 + \cos\beta\,\sigma^y_1\,,\\ \sigma^z_{N+1} &= \sigma^z_1\,.\end{aligned} \tag{1.78}$$

Notice that $\beta = 0$ corresponds to periodic boundary conditions. We propose the correction for $(u_1, u_2) = (\frac{i}{2}, -\frac{i}{2})$ as follows

$$u_1 = \frac{i}{2} + c_1\beta + O(\beta^2)\,, \;\; u_2 = -\frac{i}{2} + c_2\beta + O(\beta^2)\,, \tag{1.79}$$

(where the constants c_1, c_2 are to be determined) which again leads to the consistency condition (1.77), and also corresponding conditions for XXZ spin-$\frac{1}{2}$, XXX spin-s and XXZ spin-s.

Chapter 4: Boundary energy of the open XXX chain with a non-diagonal boundary term

R. I. Nepomechie and C. Wang, J.Phys. A47 (2014) 032001, arXiv:1310.6305 [hep-th].

For the XXX spin-$\frac{1}{2}$ chain with a nondiagonal boundary term (1.54), the new BAEs (1.69) derived from the new T-Q equation (1.66) do not have a conventional form, so are they useful? For example, can they be used to calculate the ground state energy in the thermodynamic limit $N \to \infty$? As a preliminary step, we attempt to compute the boundary energy.

For simplicity, we focus on the limit that the coefficient ξ of the non-diagonal boundary term goes to zero, and compute the leading correction (of order ξ^2) to the boundary energy. In the limit $\xi \to 0$, we find that the N Bethe roots for the ground state split evenly into two sets: "small" roots that satisfy the diagonal Bethe equations, and "large" roots that satisfy a generalization fo the Richardson-Gaudin equations. We evaluate the contribution of the two sets of roots to the leading correction of the boundary energy.

Chapter 5: Quantum group symmetries and completeness for $A_{2n}^{(2)}$ open spin chains

I. Ahmed, R. I. Nepomechie and C. Wang, submitted to J.Phys. A, arXiv:1702.01482.

It has long been known that, for one simple set of integrable boundary conditions ($K^- = I, K^+ = M$), the $A_{2n}^{(2)}$ open chains have $U_q(B_n)$ symmetry [23]. In Chapter 5, we show that open $A_{2n}^{(2)}$ chains with another set of integrable boundary conditions has $U_q(C_n)$ symmetry. (The symmetry for the case $n = 1$ was already noticed in [31].) We further show that these symmetries completely account for the multiplicities and degeneracies of the spectrum of the transfer matrices.

CHAPTER 2

Algebraic Bethe ansatz for singular solutions

2.1 Background

It is well known that the isotropic periodic spin-$\frac{1}{2}$ Heisenberg quantum spin chain with N sites, with Hamiltonian

$$H = \frac{1}{4}\sum_{n=1}^{N} \left(\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1\right) , \qquad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1 \,, \tag{2.1}$$

can be solved by algebraic Bethe ansatz (ABA): the eigenvalues are given by

$$E = -\frac{1}{2}\sum_{k=1}^{M} \frac{1}{\lambda_k^2 + \frac{1}{4}} \,, \tag{2.2}$$

and the corresponding $su(2)$ highest-weight eigenvectors are given by the Bethe vectors

$$|\lambda_1 \,, \ldots \,, \lambda_M\rangle = B(\lambda_1) \cdots B(\lambda_M)|0\rangle \,, \tag{2.3}$$

where $|0\rangle$ is the reference state with all spins up, $\{\lambda_1 \,, \ldots \,, \lambda_M\}$ are distinct and satisfy the Bethe equations

$$\left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}}\right)^N = \prod_{\substack{j \neq k \\ j=1}}^{M} \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i} \,, \qquad k = 1 \,, \cdots , M \,, \tag{2.4}$$

and $M = 0, 1, \ldots, \frac{N}{2}$. The spin s of the state is given by $s = \frac{N}{2} - M$. (See, for example, [9, 20].)

It is also well known that the so-called two-string $(\lambda_1 , \lambda_2) = (\frac{i}{2} , -\frac{i}{2})$ is an *exact* solution of the Bethe equations for $N \geq 4$. This fact is particularly easy to see from the Bethe equations in the pole-free form

$$\begin{aligned} (\lambda_1 + \frac{i}{2})^N(\lambda_1 - \lambda_2 - i) &= (\lambda_1 - \tfrac{i}{2})^N(\lambda_1 - \lambda_2 + i) \,, \\ (\lambda_2 + \frac{i}{2})^N(\lambda_2 - \lambda_1 - i) &= (\lambda_2 - \tfrac{i}{2})^N(\lambda_2 - \lambda_1 + i) \,. \end{aligned} \tag{2.5}$$

This solution is singular, as both the corresponding energy (2.2) and Bethe vector (2.3) are divergent.[1] Clearly, it is necessary to regularize this solution. The naive regularization

$$\lambda_1^{naive} = \frac{i}{2} + \epsilon \,, \qquad \lambda_2^{naive} = -\frac{i}{2} + \epsilon \tag{2.6}$$

gives the correct value of the energy in the $\epsilon \to 0$ limit, namely, $E = -1$.

What is perhaps not so well known is that this naive regularization gives a wrong result for the eigenvector.[2] Indeed, the vector $\lim_{\epsilon\to 0} \, |\lambda_1^{naive} , \lambda_2^{naive}\rangle$ is finite, but it is *not* an eigenvector of the Hamiltonian! For example, in the case $N = 4$, we easily find with `Mathematica` that

$$\lim_{\epsilon\to 0} \, |\lambda_1^{naive} , \lambda_2^{naive}\rangle = (0, 0, 0, 2, 0, 0, -2, 0, 0, 0, 0, 0, 2, 0, 0, 0) \,, \tag{2.7}$$

[1] While the divergence of the energy is obvious, the divergence of the Bethe vector is a consequence of our non-standard conventions, which we specify in Section 2.2 below. In the standard conventions, the Bethe vector would instead be null.

[2] Difficulties with constructing the eigenvector corresponding to the Bethe roots $\pm\frac{i}{2}$ were already noted in [32, 33].

while the correct eigenvector with $E=-1$ and $s=0$ is known to be instead [3]

$$(0,0,0,2,0,0,-2,0,0,-2,0,0,2,0,0,0)\,. \tag{2.9}$$

We further observe that, for general values of N, the correct eigenvector can be obtained within the ABA approach by introducing a suitable additional correction of order ϵ^N to the Bethe roots:[4]

$$\lambda_1 = \frac{i}{2} + \epsilon + c\,\epsilon^N\,, \qquad \lambda_2 = -\frac{i}{2} + \epsilon\,, \tag{2.10}$$

where the parameter c is independent of ϵ. Returning to the example of $N=4$, we find

$$\lim_{\epsilon\to 0}\, |\lambda_1\,,\lambda_2\rangle = (0,0,0,2,0,0,-2,0,0,ic,0,0,2,0,0,0)\,. \tag{2.11}$$

Comparing with (2.9), we see that the requisite value of the parameter in this case is $c=2i$.

In Section 2.2, we address the question of how to determine in a systematic way the parameter c in (2.10), which (as we have already seen) is necessary for obtaining the correct eigenvector. Clearly, it is not a matter of simply solving the Bethe equations (2.4), since they are not satisfied by (2.10) for ϵ finite. Indeed, we shall find that the Bethe equations themselves acquire ϵ-dependent corrections. These "generalized" Bethe equations (see Eq. (2.20) below) constitute our main new result. In Section

[3]For any even N, the Bethe vector corresponding to the 2-string $\pm\frac{i}{2}$ can be expressed as [34]

$$\sum_{k=1}^{N}(-1)^k S_k^- S_{k+1}^- |0\rangle\,. \tag{2.8}$$

One can easily verify that for $N=4$ this vector is indeed proportional to (2.9).

[4]Such higher-order corrections of singular Bethe roots were already noted in Eq. (3.4) of [35] and studied further in [36].

2.3, we extend this approach to general singular solutions, i.e., solutions of the Bethe equations where two of the roots are $\pm\frac{i}{2}$. Typically, there are many such solutions, but relatively few correspond to eigenvectors of the model. We find that the generalized Bethe equations provide a practical way of determining which of the singular solutions correspond to eigenvectors. Section 2.4 summarizes our main conclusions.

Singular solutions do not appear in a related model, namely, the Heisenberg chain with twisted boundary conditions. A small twist angle ϕ then plays a similar role to our parameter ϵ. This alternative approach for dealing with singular solutions is briefly considered in appendix B.3 of [37] and in section 2.1 of [38]. Since the twist breaks the $su(2)$ symmetry, the Bethe vectors are no longer highest-weight vectors. Our point of view is that the isotropic periodic Heisenberg chain for finite N is a well-defined model, and therefore should be understandable independently of other models; it is only its Bethe ansatz solution that is not completely well defined.

Yet another approach for constructing the Bethe vectors corresponding to singular solutions, involving Sklyanin's separation of variables, was carefully analyzed in [39].

2.2 Determining the parameter

We begin by briefly establishing our conventions. Following [9], the R-matrix is given by

$$R_{a_1a_2}(\lambda) = \lambda\mathbb{I}_{a_1a_2} + i\mathcal{P}_{a_1a_2}\,, \tag{2.12}$$

where $\mathbb{I}$ and $\mathcal{P}$ are the 4×4 identity and permutation matrices, respectively. However, as explained below, we choose a different normalization for the Lax operator, namely,

$$L_{na}(\lambda) = \frac{1}{(\lambda + \frac{i}{2})} \left[(\lambda - \frac{i}{2})\mathbb{I}_{na} + i\mathcal{P}_{na} \right] \,, \tag{2.13}$$

which diverges for $\lambda = -\frac{i}{2}$. As usual, the monodromy matrix is given by

$$T_a(\lambda) = L_{Na}(\lambda) \cdots L_{1a}(\lambda) = \left(\begin{array}{cc} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{array} \right) \,, \tag{2.14}$$

and the transfer matrix is given by

$$t(\lambda) = \mathrm{tr}_a\, T_a(\lambda) = A(\lambda) + D(\lambda)\,. \tag{2.15}$$

The reference state is denoted by $|0\rangle = \binom{1}{0}^{\otimes N}$.

We next recall the action of the transfer matrix on an off-shell Bethe vector (2.3) [9]

$$\begin{aligned} t(\lambda)|\lambda_1\,, \ldots\,, \lambda_M\rangle &= \Lambda(\lambda)|\lambda_1\,, \ldots\,, \lambda_M\rangle \\ &+ \sum_{k=1}^{M} F_k(\lambda, \{\lambda\}) B(\lambda_1) \cdots \widehat{B}(\lambda_k) \cdots B(\lambda_M) B(\lambda)|0\rangle\,, \end{aligned} \tag{2.16}$$

where a hat is used to denote an operator that is omitted, and

$$\Lambda(\lambda) = \prod_{j=1}^{M} \left(\frac{\lambda - \lambda_j - i}{\lambda - \lambda_j} \right) + \left(\frac{\lambda - \frac{i}{2}}{\lambda + \frac{i}{2}} \right)^N \prod_{j=1}^{M} \left(\frac{\lambda - \lambda_j + i}{\lambda - \lambda_j} \right)\,, \tag{2.17}$$

$$F_k(\lambda, \{\lambda\}) = \frac{i}{\lambda - \lambda_k} \left[\prod_{j \ne k}^{M} \left(\frac{\lambda_k - \lambda_j - i}{\lambda_k - \lambda_j} \right) - \left(\frac{\lambda_k - \frac{i}{2}}{\lambda_k + \frac{i}{2}} \right)^N \prod_{j \ne k}^{M} \left(\frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j} \right) \right]\,. \tag{2.18}$$

The Bethe equations (2.4) are precisely the conditions $F_k(\lambda, \{\lambda\}) = 0$, which ensure that the "unwanted" terms vanish, in which case the Bethe vector $|\lambda_1\,, \ldots\,, \lambda_M\rangle$ is an eigenvector of the transfer matrix $t(\lambda)$, with corresponding eigenvalue $\Lambda(\lambda)$ given by

(2.17). In particular, for $M = 2$, the relation (2.16) reduces to

$$t(\lambda)|\lambda_1\,,\lambda_2\rangle = \Lambda(\lambda)|\lambda_1\,,\lambda_2\rangle + F_1(\lambda,\{\lambda\})B(\lambda_2)B(\lambda)|0\rangle + F_2(\lambda,\{\lambda\})B(\lambda_1)B(\lambda)|0\rangle\,, \tag{2.19}$$

which holds for generic values of $\lambda\,,\lambda_1$ and λ_2.

Let us now focus on the special case of the two-string solution $\pm\frac{i}{2}$. As already mentioned in the Introduction, the corresponding Bethe vector $|\frac{i}{2},-\frac{i}{2}\rangle$ is singular: some of its components have the form 0/0. (If we had defined the Lax operator (2.13) without dividing by $(\lambda+\frac{i}{2})$ as in [9], then the corresponding Bethe vector would instead be null [32].) In particular, the creation operator $B(\frac{i}{2})$ is finite, but $B(-\frac{i}{2})$ is singular.

Let us first consider the naive regularization (2.6). The key observation is that, for $\epsilon \to 0$, the most singular matrix elements of $B(\lambda_2^{naive})$ are of order $\frac{1}{\epsilon^N}$. (See (2.38).) It follows from the off-shell relation (2.19) that, for $\epsilon \to 0$, the coefficients F_1 and F_2 must satisfy

$$F_1(\lambda,\{\lambda\}) \sim \epsilon^{N+1}\,, \qquad F_2(\lambda,\{\lambda\}) \sim \epsilon\,, \tag{2.20}$$

in order that the Bethe vector $\lim_{\epsilon\to 0}\ |\lambda_1^{naive}\,,\lambda_2^{naive}\rangle$ be an eigenvector of the transfer matrix. However, explicit computation using (2.6) shows that $F_1(\lambda,\{\lambda\}) \sim \epsilon^N$ (instead of ϵ^{N+1}) and $F_2(\lambda,\{\lambda\}) \sim 1$ (instead of ϵ). Hence, the "unwanted" terms in (2.19) are finite (do not vanish), which explains why the corresponding Bethe vector is not an eigenvector.[5]

[5]The fact that $B(\lambda_2^{naive})$ has matrix elements of order $\frac{1}{\epsilon^N}$ suggests that $|\lambda_1^{naive}\,,\lambda_2^{naive}\rangle \sim \frac{1}{\epsilon^N}$. However, as shown in the Appendix, this vector is finite for $\epsilon \to 0$.

Let us therefore consider the regularization (2.10). The leading behavior of $B(\lambda_1)$ and $B(\lambda_2)$ as $\epsilon \to 0$ remains the same as with the naive regularization; i.e., $B(\lambda_1) \sim \frac{1}{\epsilon^N}$ and $B(\lambda_2) \sim 1$. Hence, the conditions (2.20) must still be satisfied to ensure that the Bethe vector is an eigenvector of the transfer matrix. Explicit computation using (2.10) gives

$$\begin{aligned} F_1(\lambda, \{\lambda\}) &= \left(\frac{c + 2i^{-(N+1)}}{\lambda - \frac{i}{2}}\right) \epsilon^N + O(\epsilon^{N+1}) \,, \\ F_2(\lambda, \{\lambda\}) &= \left(\frac{2i - i^{-N} c}{\lambda + \frac{i}{2}}\right) + O(\epsilon) \,. \end{aligned} \tag{2.21}$$

For even N, both conditions (2.20) can be satisfied by setting

$$c = 2i(-1)^{N/2} \,, \tag{2.22}$$

which reproduces our earlier result for $N = 4$ (see below Eq. (2.11)). We have also explicitly verified that, for $N = 6$, the ABA Bethe vector constructed using (2.10) and (2.22) is indeed an eigenvector of the Hamiltonian.[6] Interestingly, the two conditions (2.20) cannot be simultaneously satisfied for odd N, implying that the two-string $\pm\frac{i}{2}$ is *not* a bona fide solution for odd N.[7]

We note that the regularization (2.10) can be slightly generalized. Indeed, we can introduce a two-parameter regularization

$$\lambda_1 = \frac{i}{2} + \epsilon + c_1\, \epsilon^N \,, \qquad \lambda_2 = -\frac{i}{2} + \epsilon + c_2\, \epsilon^N \,. \tag{2.23}$$

The conditions (2.20) now imply (for even N) that

$$c_1 - c_2 = 2i(-1)^{N/2} \,. \tag{2.24}$$

[6] It was claimed in [33] that the Bethe ansatz fails for this case.

[7] For $N = 5$, the Clebsch-Gordan theorem implies that there are five highest-weight eigenvectors with $s = \frac{1}{2}$; and we have explicitly verified that all of these eigenvectors can be constructed with Bethe roots other than $\pm\frac{i}{2}$, thereby directly proving that the solution $\pm\frac{i}{2}$ must be discarded.

For finite ϵ, the corresponding energy (2.2) depends only on the difference $c_1 - c_2$. If we impose the additional constraint $\lambda_1 = \lambda_2^*$ [40], then we obtain $c_1 = c_2^* = i(-1)^{N/2}$. In short, for even N, a regularization of the singular solution $\pm\frac{i}{2}$ that produces the correct eigenvector in the $\epsilon \to 0$ limit, and also satisfies $\lambda_1 = \lambda_2^*$, is given by

$$\lambda_1 = \frac{i}{2} + \epsilon + i(-1)^{N/2}\,\epsilon^N\,, \qquad \lambda_2 = -\frac{i}{2} + \epsilon - i(-1)^{N/2}\,\epsilon^N\,. \tag{2.25}$$

2.3 General singular solutions

We now consider a general singular solution of the Bethe equations, which has the form

$$\{\frac{i}{2}\,, -\frac{i}{2}\,, \lambda_3\,, \ldots\,, \lambda_M\}\,, \tag{2.26}$$

where $\lambda_3\,, \ldots\,, \lambda_M$ are distinct and are not equal to $\pm\frac{i}{2}$. Proceeding as before, we regularize the first two roots as in Eq. (2.10). The Bethe equations (2.4) imply that the last $M-2$ roots $\{\lambda_3\,, \ldots\,, \lambda_M\}$ obey

$$\left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}}\right)^{N-1} \left(\frac{\lambda_k - \frac{3i}{2}}{\lambda_k + \frac{3i}{2}}\right) = \prod_{\substack{j\neq k\\ j=3}}^{M} \frac{\lambda_k - \lambda_j + i}{\lambda_k - \lambda_j - i}\,, \qquad k = 3\,, \cdots\,, M\,. \tag{2.27}$$

We again impose the two generalized Bethe equations

$$F_1(\lambda, \{\lambda\}) \sim \epsilon^{N+1}\,, \qquad F_2(\lambda, \{\lambda\}) \sim \epsilon\,, \tag{2.28}$$

where F_k is defined in (2.18). The equations (2.28) ensure that the Bethe vector corresponding to the singular solution (2.26), namely

$$\lim_{\epsilon\to 0}\, |\lambda_1\,, \ldots\,, \lambda_M\rangle\,, \tag{2.29}$$

where λ_1 , λ_2 are given by (2.10) and $|\lambda_1 , \dots , \lambda_M\rangle$ is given by (2.3), is an eigenvector of the transfer matrix.

In other words, given a solution $\{\lambda_3 , \dots , \lambda_M\}$ of (2.27), if the equations (2.28) *can* be satisfied, then they determine the parameter c in (2.10), and the corresponding Bethe vector (2.29) is an eigenvector of the transfer matrix. We call such a singular solution "physical". On the other hand, if the equations (2.28) *cannot* be satisfied, then – despite the fact that the usual Bethe equations (2.4), (2.27) are obeyed – this solution cannot be used to construct an eigenvector of the transfer matrix. We call such a singular solution "unphysical". Hence, according to the previous section, all singular solutions with odd N and $M = 2$ are unphysical.

Eqs. (2.28) can be simplified as follows. Using (2.10), we find that these two equations imply

$$c = -\frac{2}{i^{N+1}} \prod_{j=3}^{M} \frac{\lambda_j - \frac{3i}{2}}{\lambda_j + \frac{i}{2}} \,, \qquad c = 2 i^{N+1} \prod_{j=3}^{M} \frac{\lambda_j + \frac{3i}{2}}{\lambda_j - \frac{i}{2}} \,, \tag{2.30}$$

respectively. These equations in turn imply the consistency condition

$$\prod_{j=3}^{M} \left(\frac{\lambda_j - \frac{i}{2}}{\lambda_j + \frac{i}{2}}\right) \left(\frac{\lambda_j - \frac{3i}{2}}{\lambda_j + \frac{3i}{2}}\right) = (-1)^N \,. \tag{2.31}$$

By forming the product of all the Bethe equations (2.27), we obtain the relation

$$\prod_{k=3}^{M} \left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}}\right)^{N-1} \left(\frac{\lambda_k - \frac{3i}{2}}{\lambda_k + \frac{3i}{2}}\right) = 1 \,, \tag{2.32}$$

using which the consistency condition (2.31) takes the simple form

$$\left[- \prod_{k=3}^{M} \left(\frac{\lambda_k + \frac{i}{2}}{\lambda_k - \frac{i}{2}}\right) \right]^N = 1 \,. \tag{2.33}$$

We remark that the condition (2.33) provides a practical way to select from among the many singular solutions of the Bethe equations (2.27) the physically relevant subset, which is generally much smaller. For example, for $N = 6$ and $M = 3$, the Bethe equations (2.4), (2.27) have 5 singular solutions, of which only one is physical. Similarly, for $N = 8$ and $M = 4$, we find 21 singular solutions, of which only 3 are physical.[8]

2.4 Conclusion

We have seen that the ABA for the isotropic periodic Heisenberg chain must be extended for solutions of the Bethe equations containing $\pm\frac{i}{2}$. Indeed, such singular solutions must be carefully regularized as in (2.10) or (2.23). This regularization involves a parameter that can be determined using a generalization of the Bethe equations given by (2.20), where F_k is defined in (2.18). These equations also provide a practical way of determining which singular solutions correspond to eigenvectors of the model. In particular, the solution $\pm\frac{i}{2}$ must be excluded for odd N.

It would be interesting to know whether the finite-ϵ corrections to the energy have any physical significance. We expect that our analysis can be extended to the anisotropic case.

Note Added

After completing this work, we became aware of [42], where similar results were obtained for the solution $\pm\frac{i}{2}$. However, our approach differs significantly from theirs.

[8] The number of singular states of the XXZ chain are estimated in [41].

2.5 Appendix

Here we fill in some details. It is convenient to define an unrenormalized Lax operator (as in [9]):

$$\tilde{L}_{na}(\lambda) = (\lambda - \frac{i}{2})\mathbb{I}_{na} + i\mathcal{P}_{na}\,, \tag{2.34}$$

and correspondingly

$$\tilde{T}_a(\lambda) = \tilde{L}_{Na}(\lambda)\cdots\tilde{L}_{1a}(\lambda) = \begin{pmatrix} \tilde{A}(\lambda) & \tilde{B}(\lambda) \\ \tilde{C}(\lambda) & \tilde{D}(\lambda) \end{pmatrix}. \tag{2.35}$$

Evidently,

$$L_{na}(\lambda) = \frac{1}{(\lambda + \frac{i}{2})}\,\tilde{L}_{na}(\lambda)\,, \qquad T_a(\lambda) = \frac{1}{(\lambda + \frac{i}{2})^N}\,\tilde{T}_a(\lambda)\,. \tag{2.36}$$

In particular,

$$B(\lambda) = \frac{1}{(\lambda + \frac{i}{2})^N}\,\tilde{B}(\lambda)\,. \tag{2.37}$$

Since $\tilde{B}(\pm\frac{i}{2})$ are finite, it follows that $B(\frac{i}{2})$ is also finite, and

$$B(-\frac{i}{2} + \epsilon) \sim \frac{1}{\epsilon^N} \tag{2.38}$$

plus less singular terms.

The fact (2.38) suggests that $|\lambda_1^{naive}, \lambda_2^{naive}\rangle = B(\frac{i}{2}+\epsilon)\,B(-\frac{i}{2}+\epsilon)|0\rangle$ should be similarly divergent for $\epsilon \to 0$. However, we shall now argue that this vector is in fact finite. In view of (2.37), it suffices to show that[9]

$$\tilde{B}(\frac{i}{2} + \epsilon)\,\tilde{B}(-\frac{i}{2} + \epsilon)|0\rangle \sim \epsilon^N\,. \tag{2.39}$$

[9]The result (2.39) implies, as already noted, that this vector is null in the limit $\epsilon \to 0$.

To this end, we proceed by induction. The behavior (2.39) can be easily verified explicitly for $N = 4$ using `Mathematica`. We observe from (2.35) that the monodromy matrices for $N-1$ and N sites are related by

$$\tilde{T}_a^{(N)}(\lambda) = \tilde{L}_{Na}(\lambda)\,\tilde{T}_a^{(N-1)}(\lambda)\,, \tag{2.40}$$

which implies that

$$\begin{pmatrix} \tilde{A}^{(N)}(\lambda) & \tilde{B}^{(N)}(\lambda) \\ \tilde{C}^{(N)}(\lambda) & \tilde{D}^{(N)}(\lambda) \end{pmatrix} = \begin{pmatrix} \tilde{a}_N(\lambda) & \tilde{b}_N(\lambda) \\ \tilde{c}_N(\lambda) & \tilde{d}_N(\lambda) \end{pmatrix} \begin{pmatrix} \tilde{A}^{(N-1)}(\lambda) & \tilde{B}^{(N-1)}(\lambda) \\ \tilde{C}^{(N-1)}(\lambda) & \tilde{D}^{(N-1)}(\lambda) \end{pmatrix}, \tag{2.41}$$

where

$$\begin{aligned} \tilde{a}_N(\lambda) &= \begin{pmatrix} \lambda + \frac{i}{2} & 0 \\ 0 & \lambda - \frac{i}{2} \end{pmatrix}, \qquad \tilde{b}_N(\lambda) = \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix}, \\ \tilde{c}_N(\lambda) &= \begin{pmatrix} 0 & i \\ 0 & 0 \end{pmatrix}, \qquad \tilde{d}_N(\lambda) = \begin{pmatrix} \lambda - \frac{i}{2} & 0 \\ 0 & \lambda + \frac{i}{2} \end{pmatrix}. \end{aligned} \tag{2.42}$$

In particular,

$$\tilde{B}^{(N)}(\lambda) = \tilde{a}_N(\lambda)\,\tilde{B}^{(N-1)}(\lambda) + \tilde{b}_N(\lambda)\,\tilde{D}^{(N-1)}(\lambda)\,. \tag{2.43}$$

It follows that

$$\begin{aligned}
\tilde{B}^{(N)}(\lambda_1)\,\tilde{B}^{(N)}(\lambda_2)|0\rangle^{(N)} &= \left[\tilde{a}_N(\lambda_1)\,\tilde{B}^{(N-1)}(\lambda_1) + \tilde{b}_N(\lambda_1)\,\tilde{D}^{(N-1)}(\lambda_1)\right] \\
&\times \left[\tilde{a}_N(\lambda_2)\,\tilde{B}^{(N-1)}(\lambda_2) + \tilde{b}_N(\lambda_2)\,\tilde{D}^{(N-1)}(\lambda_2)\right]|0\rangle^{(N-1)}\begin{pmatrix}1\\0\end{pmatrix}_N \\
&= \Bigg[\tilde{a}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\,\tilde{B}^{(N-1)}(\lambda_1)\,\tilde{B}^{(N-1)}(\lambda_2) \\
&\quad + \tilde{a}_N(\lambda_1)\,\tilde{b}_N(\lambda_2)\,\tilde{B}^{(N-1)}(\lambda_1)\,\tilde{D}^{(N-1)}(\lambda_2) \\
&\quad + \tilde{b}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\,\tilde{D}^{(N-1)}(\lambda_1)\,\tilde{B}^{(N-1)}(\lambda_2) \\
&\quad + \tilde{b}_N(\lambda_1)\,\tilde{b}_N(\lambda_2)\,\tilde{D}^{(N-1)}(\lambda_1)\,\tilde{D}^{(N-1)}(\lambda_2)\Bigg]|0\rangle^{(N-1)}\begin{pmatrix}1\\0\end{pmatrix}_N
\end{aligned} \tag{2.44}$$

for $\lambda_1\,,\lambda_2$ arbitrary.

We now set $\lambda_1 = \lambda_1^{naive} = \frac{i}{2} + \epsilon$ and $\lambda_2 = \lambda_2^{naive} = -\frac{i}{2} + \epsilon$, and we consider the four terms on the RHS of (2.44), starting with the first: by the induction hypothesis,

$$\tilde{B}^{(N-1)}(\lambda_1)\,\tilde{B}^{(N-1)}(\lambda_2)|0\rangle^{(N-1)} \sim \epsilon^{N-1}\,. \tag{2.45}$$

Moreover, it is easy to see that

$$\tilde{a}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\begin{pmatrix}1\\0\end{pmatrix}_N \sim \epsilon\,. \tag{2.46}$$

Hence, the first term on the RHS of (2.44) is of order ϵ^N.

The fourth term on the RHS of (2.44) is zero because

$$\tilde{b}_N(\lambda_1)\,\tilde{b}_N(\lambda_2)\begin{pmatrix}1\\0\end{pmatrix}_N = 0\,. \tag{2.47}$$

Using the exchange relation [9]

$$\tilde{D}(\lambda_1)\,\tilde{B}(\lambda_2) = \frac{\lambda_1 - \lambda_2 + i}{\lambda_1 - \lambda_2}\tilde{B}(\lambda_2)\,\tilde{D}(\lambda_1) - \frac{i}{\lambda_1 - \lambda_2}\tilde{B}(\lambda_1)\,\tilde{D}(\lambda_2) \tag{2.48}$$

in the third term, we see that the second and third terms on the RHS of (2.44) combine to give

$$\Big\{ \left[\tilde{a}_N(\lambda_1)\,\tilde{b}_N(\lambda_2) - \tilde{b}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\right] \tilde{B}^{(N-1)}(\lambda_1)\,\tilde{D}^{(N-1)}(\lambda_2)$$

$$+ 2\tilde{b}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\tilde{B}^{(N-1)}(\lambda_2)\,\tilde{D}^{(N-1)}(\lambda_1) \Big\} |0\rangle^{(N-1)} \binom{1}{0}_N \tag{2.49}$$

The first line of (2.49) gives a vanishing contribution because

$$\left[\tilde{a}_N(\lambda_1)\,\tilde{b}_N(\lambda_2) - \tilde{b}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\right] \binom{1}{0}_N = 0\,. \tag{2.50}$$

The second line of (2.49) is of order ϵ^N, since

$$\tilde{D}^{(N-1)}(\lambda_1)|0\rangle^{(N-1)} \sim \epsilon^{N-1}\,, \tag{2.51}$$

and

$$\tilde{b}_N(\lambda_1)\,\tilde{a}_N(\lambda_2)\binom{1}{0}_N \sim \epsilon\,. \tag{2.52}$$

In short, we have shown that

$$\tilde{B}^{(N)}(\lambda_1)\,\tilde{B}^{(N)}(\lambda_2)|0\rangle^{(N)} \sim \epsilon^N\,, \tag{2.53}$$

which concludes the inductive proof of our claim (2.39).

CHAPTER 3

Twisting singular solutions of Bethe's equations

3.1 Background

The periodic spin-1/2 isotropic Heisenberg (XXX) quantum spin chain, whose Hamiltonian is given by[1]

$$H = \frac{1}{4}\sum_{n=1}^{N}\left(\vec{\sigma}_n \cdot \vec{\sigma}_{n+1} - 1\right) , \qquad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1 \, , \tag{3.1}$$

is well known to be solvable by Bethe ansatz: both the eigenvectors and the eigenvalues of the Hamiltonian can be expressed in terms of solutions of the Bethe equa-

[1]We denote by $\vec{\sigma} = (\sigma^x \, , \sigma^y \, , \sigma^z)$ the standard Pauli spin matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} ,$$

which act on a two-dimensional complex vector space $V = \mathcal{C}^2$. Moreover, σ^i_n denotes an operator on the N-fold tensor product space $V^{\otimes N}$, which acts as σ^i on the n^{th} copy of V, and as the identity operator otherwise

$$\sigma^i_n = \mathbb{I} \otimes \cdots \otimes \mathbb{I} \otimes \overset{\overset{n}{\downarrow}}{\sigma^i} \otimes \mathbb{I} \cdots \otimes \mathbb{I} \, ,$$

where here $\mathbb{I}$ denotes the 2×2 identity matrix.

tions [9,13]

$$\left(\frac{\lambda_j+\frac{i}{2}}{\lambda_j-\frac{i}{2}}\right)^N=\prod_{\substack{k\neq j\\k=1}}^{M}\frac{\lambda_j-\lambda_k+i}{\lambda_j-\lambda_k-i}\,,\qquad j=1,\ldots,M\,,\qquad M=0,1,\ldots,\frac{N}{2}\,. \tag{3.2}$$

Indeed, the eigenvectors are given in terms of the "Bethe roots" $\{\lambda_j\}$ by the Bethe vector

$$\prod_{j=1}^{M}B(\lambda_j)|0\rangle\,, \tag{3.3}$$

where $B(\lambda)$ is a certain creation operator[2] and $|0\rangle$ is the state with all N spins up; and the corresponding eigenvalues are given by

$$E=-\frac{1}{2}\sum_{j=1}^{M}\frac{1}{\lambda_j^2+\frac{1}{4}}\,. \tag{3.4}$$

It is also well known that the Bethe equations admit so-called singular (or exceptional) solutions, for which the corresponding eigenvectors and eigenvalues are ill-defined. (See e.g. [32,34–38,41–46].) The simplest example occurs for $M=2$ and any $N\geq 4$, namely $(\lambda_1,\lambda_2)=(i/2\,,-i/2)$. To see that this is an exact solution, it is convenient to rewrite the Bethe equations (3.2) in polynomial form (see e.g. (3.10) below). The corresponding energy (3.4) is evidently ill-defined, and the corresponding eigenvector (3.3) can be shown to be null.

A general singular solution of the Bethe equations has the form

$$\{\frac{i}{2}\,,-\frac{i}{2}\,,\lambda_3\,,\ldots\,,\lambda_M\}\,, \tag{3.5}$$

[2] We remind the reader that the monodromy matrix is given by [9]

$$T_a(\lambda)=L_{Na}(\lambda)\cdots L_{1a}(\lambda)=\begin{pmatrix}A(\lambda) & B(\lambda)\\ C(\lambda) & D(\lambda)\end{pmatrix}\,,$$

where the Lax operator is $L_{na}(\lambda)=(\lambda-\frac{i}{2})\mathbb{I}_{na}+i\mathcal{P}_{na}$, and $\mathcal{P}$ is the permutation matrix on $V\otimes V$. The operator $B(\lambda)$ serves as a creation operator for constructing the eigenstates of H, and has the property $[B(\lambda)\,,B(\lambda')]=0$. The transfer matrix $t(\lambda)=\mathrm{tr}_a\,T_a(\lambda)=A(\lambda)+D(\lambda)$ satisfies $[t(\lambda)\,,t(\lambda')]=0$, and therefore is the generator of commuting quantities $H_n=\frac{i}{2}\frac{d^n}{d\lambda^n}\log t(\lambda)|_{\lambda=\frac{i}{2}}$, with $H=H_1-\frac{N}{2}$.

where $\lambda_3\,, \ldots\,, \lambda_M$ are distinct and not equal to $\pm i/2$. A solution that does not contain $\pm i/2$ is called regular. Note that the order of the Bethe roots does not matter, since the Bethe equations (3.2) as well as the eigenvectors (3.3) and eigenvalues (3.4) are invariant under any permutation of $\{\lambda_1\,, \ldots\,, \lambda_M\}$.

It is important to recognize that there are two main types of singular solutions: **physical** singular solutions (which correspond to genuine eigenvalues and eigenvectors of the Hamiltonian), and **unphysical** singular solutions (which do not correspond to eigenvalues and eigenvectors of the Hamiltonian). The simplest example of the former is $\pm i/2$ for N even, while the simplest example of the latter is $\pm i/2$ for N odd.

We have argued in [46] that a general singular solution (3.5) is physical if $\lambda_3, \ldots, \lambda_M$ satisfy the following additional condition

$$\left[-\prod_{j=3}^{M}\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)\right]^N = 1\,. \tag{3.6}$$

For the case $M = 2$, this condition reduces to the requirement (already noted above) that N should be even.

This condition was used in [47] to explicitly demonstrate the completeness of the solutions of Bethe's equations up to $N = 14$. That is, the number of regular solutions plus the number of physical singular solutions (i.e., those singular solutions that satisfy (3.6)) exactly coincides with the number needed to account for all 2^N eigenstates of the model. For further discussions of the completeness problem, see for example [9, 13, 39, 44, 48–55].

For the integrable spin-s XXX chain, a generalization of (3.6) was derived and used to investigate completeness in [56]. For related recent developments, see [57–59].

The derivation of the constraint (3.6) in [46] (and similarly of its spin-s generalization in [56]) relies on regularizing the singular solution (3.5) by replacing the first two roots by

$$\lambda_1 = \frac{i}{2} + \epsilon + c\,\epsilon^N\,, \qquad \lambda_2 = -\frac{i}{2} + \epsilon\,, \tag{3.7}$$

where ϵ is a small parameter, and c is a constant that is still to be determined. This way of regularizing a singular solution was considered previously in [35, 36, 42, 44]. Requiring that the corresponding Bethe vector (constructed as in (3.3), except with a different normalization of the creation operators, namely $B(\lambda) \mapsto (\lambda + \frac{i}{2})^{-N} B(\lambda)$, which diverges at $\lambda = -\frac{i}{2}$) be an eigenvector of the transfer matrix in the limit $\epsilon \to 0$ gives rise to two equations for the constant c, whose consistency implies (3.6).

The regularization scheme (3.7) may be rightly criticized as being somewhat unphysical and ad-hoc. Moreover, one can worry that a different choice of regularization could lead to a result different from (3.6). The primary motivation for the present work was to see whether this constraint could be derived using a different, and more physical, regularization.

An alternative regularization is to introduce a small diagonal twist angle β in the boundary conditions (see e.g. [43])

$$\begin{aligned}
\sigma^x_{N+1} &= \cos\beta\,\sigma^x_1 - \sin\beta\,\sigma^y_1\,, \\
\sigma^y_{N+1} &= \sin\beta\,\sigma^x_1 + \cos\beta\,\sigma^y_1\,, \\
\sigma^z_{N+1} &= \sigma^z_1\,.
\end{aligned} \tag{3.8}$$

This boundary condition evidently breaks the $SU(2)$ symmetry down to $U(1)$, and reduces to periodic boundary conditions when $\beta = 0$.

This way of regularizing a singular solution was considered previously in [32, 37, 38, 45]. Moreover, such twists have been widely used in related contexts (see e.g. [45, 50–52, 60–62] and references therein). Like (3.7), the twist regularization (3.8) involves introducing an additional parameter; however, the latter regularization is arguably more physical, since its parameter has a physical meaning.

We show here that the constraint (3.6) can indeed be derived (in fact, more easily) using the twist (3.8) as a regulator. The argument easily generalizes to the case of arbitrary spin s, and also to the XXZ case.

3.2 XXX

For the spin-1/2 XXX spin chain with twisted boundary conditions (3.8), the Bethe equations are given by

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)^N = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}\,, \qquad j = 1, \ldots, M\,, \tag{3.9}$$

which can be rewritten in polynomial form as

$$\left(\lambda_j + \frac{i}{2}\right)^N \prod_{\substack{k \neq j \\ k=1}}^{M} (\lambda_j - \lambda_k - i) = e^{-i\beta} \left(\lambda_j - \frac{i}{2}\right)^N \prod_{\substack{k \neq j \\ k=1}}^{M} (\lambda_j - \lambda_k + i)\,, \quad j = 1, \ldots, M\,. \tag{3.10}$$

We assume that, for small β, the roots $\pm i/2$ of a physical singular solution (3.5) acquire corrections of order β,[3]

$$\begin{aligned} \lambda_1 &= \tfrac{i}{2} + c_1\beta + O(\beta^2)\,, \\ \lambda_2 &= -\tfrac{i}{2} + c_2\beta + O(\beta^2)\,, \end{aligned} \tag{3.11}$$

[3] The twisted equations (3.10) evidently still admit solutions with $\pm i/2$ (i.e., without any β-dependent corrections). However, such singular solutions are unphysical.

where c_1 and c_2 are some constants (independent of β). The Bethe equations (3.10) for λ_1 and λ_2 are

$$\left(\lambda_1 + \frac{i}{2}\right)^N (\lambda_1 - \lambda_2 - i) \prod_{k=3}^{M} (\lambda_1 - \lambda_k - i) = e^{-i\beta} \left(\lambda_1 - \frac{i}{2}\right)^N (\lambda_1 - \lambda_2 + i) \prod_{k=3}^{M} (\lambda_1 - \lambda_k + i) \,,$$
$$\left(\lambda_2 + \frac{i}{2}\right)^N (\lambda_2 - \lambda_1 - i) \prod_{k=3}^{M} (\lambda_2 - \lambda_k - i) = e^{-i\beta} \left(\lambda_2 - \frac{i}{2}\right)^N (\lambda_2 - \lambda_1 + i) \prod_{k=3}^{M} (\lambda_2 - \lambda_k + i) \,.$$

Substituting (3.11), one can see that these equations are satisfied to first order in β provided that

$$c_1 = c_2 \,. \tag{3.12}$$

Forming the product of all M Bethe equations (3.9), we obtain

$$\left(\frac{\lambda_1 + \frac{i}{2}}{\lambda_1 - \frac{i}{2}} \frac{\lambda_2 + \frac{i}{2}}{\lambda_2 - \frac{i}{2}} \prod_{j=3}^{M} \frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \right)^N = e^{-iM\beta} \,. \tag{3.13}$$

Substituting (3.11) and (3.12) into (3.13) and taking the limit $\beta \to 0$, we arrive at the constraint (3.6)

$$\left[- \prod_{j=3}^{M} \left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \right) \right]^N = 1 \,. \tag{3.14}$$

This concludes our argument for the spin-1/2 XXX case. Of course, $\{\lambda_3, \ldots, \lambda_M\}$ must also obey

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \right)^{N-1} \left(\frac{\lambda_j - \frac{3i}{2}}{\lambda_j + \frac{3i}{2}} \right) = \prod_{\substack{k \neq j \\ k=3}}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i} \,, \qquad j = 3 \,, \cdots \,, M \,, \tag{3.15}$$

which follow from the Bethe equations (3.9) with $j = 3, \ldots, M$ after substituting (3.11) and taking $\beta \to 0$.

The constraint (3.14) can also be derived in a similar way using the original regularization (3.7) simply by substituting into (3.13) (with $\beta = 0$) and taking the limit $\epsilon \to 0$. This argument (which was overlooked in [46]) evidently does not require the $c\epsilon^N$ term in (3.7). However, this $c\epsilon^N$ term is needed to construct the correct eigenvector.

In order to construct the eigenvector corresponding to a physical singular solution using the twist regularization, we expect (based on [46]) that it is necessary to determine the corrections of the singular solution up to order β^N, to renormalize the Bethe vector (3.3) by the factor $1/\beta^N$, and then take the limit $\beta \to 0$. The required corrections of the singular solution can be obtained (for given explicit values $\{\lambda_j^{(0)}\}$ of $\{\lambda_3, \ldots, \lambda_M\}$ that satisfy (3.14) and (3.15)) by assuming that all the Bethe roots can be expanded in powers of β,

$$\lambda_j = \lambda_j^{(0)} + \sum_{l=1}^{N} c_j^{(l)} \beta^l + O(\beta^{N+1}) \,, \qquad j = 1\,, \ldots\,, M\,, \tag{3.16}$$

and solving the Bethe equations (3.10), (3.13) for the coefficients $c_j^{(l)}$. For example, for the simplest case $(N, M) = (4, 2)$, we find in this way

$$\begin{aligned} \lambda_1 &= \tfrac{i}{2} + \tfrac{\beta}{4} - \tfrac{\beta^3}{96} + \tfrac{i\beta^4}{256} + O(\beta^5)\,, \\ \lambda_2 &= -\tfrac{i}{2} + \tfrac{\beta}{4} - \tfrac{\beta^3}{96} - \tfrac{i\beta^4}{256} + O(\beta^5)\,. \end{aligned} \tag{3.17}$$

Moreover, we have verified by explicit computation that the vector

$$\lim_{\beta \to 0} \frac{1}{\beta^4} B(\lambda_1)\, B(\lambda_2) |0\rangle \tag{3.18}$$

is indeed proportional to the correct eigenvector [34, 42] $\sum_{k=1}^{4} (-1)^k S_k^- S_{k+1}^- |0\rangle$.

3.2.1 Spin s

Similar arguments can be applied to the integrable spin-s XXX chain with twisted boundary conditions, for arbitrary spin $s = \frac{1}{2}, 1, \frac{3}{2}, \ldots$. The Bethe equations are given by

$$\left(\frac{\lambda_j + is}{\lambda_j - is}\right)^N = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}\,, \qquad j = 1, \ldots, M\,, \tag{3.19}$$

When $\beta = 0$, these equations have singular solutions of the form [56]

$$\{is\,, i(s-1)\,, \ldots\,, -i(s-1)\,, -is\,, \lambda_{2s+2}\,, \ldots, \lambda_M\}\,, \tag{3.20}$$

where all the roots are assumed to be distinct. That is, a singular solution contains an exact string of length $2s+1$ centered at the origin.

We assume that, for small β, the roots $\{is\,, i(s-1)\,, \ldots\,, -i(s-1)\,, -is\}$ of a physical singular solution acquire corrections of order β,

$$\lambda_k \;\;= i(s+1-k) + c_k\beta + O(\beta^2)\,, \qquad k = 1\,, 2\,, \ldots\,, 2s+1\,, \tag{3.21}$$

where $\{c_k\}$ are some constants. Substituting (3.21) into the first $2s+1$ Bethe equations (i.e., Eq. (3.19) for $j = 1\,, \ldots\,, 2s+1$), we see that these equations are satisfied to first order in β provided that all the c_k's are equal,

$$c_1 = c_2 = \ldots = c_{2s+1}\,. \tag{3.22}$$

The product of all M Bethe equations (3.19) gives

$$\left(\frac{\lambda_1 + is}{\lambda_1 - is}\frac{\lambda_2 + is}{\lambda_2 - is}\cdots\frac{\lambda_{2s+1} + is}{\lambda_{2s+1} - is}\prod_{j=2s+2}^{M}\frac{\lambda_j + is}{\lambda_j - is}\right)^N = e^{-iM\beta}\,. \tag{3.23}$$

Substituting (3.21) and (3.22) into (3.23) and taking the limit $\beta \to 0$, we obtain the constraint

$$\left[(-1)^{2s}\prod_{j=2s+2}^{M}\left(\frac{\lambda_j + is}{\lambda_j - is}\right)\right]^N = 1\,. \tag{3.24}$$

This necessary condition for the singular solution (3.20) to be physical, which is evidently a generalization of the $s = 1/2$ result (3.14), was first obtained in [56] using instead a generalization of the regularization (3.7). Of course, $\{\lambda_{2s+2}, \ldots, \lambda_M\}$ must also obey

$$\left(\frac{\lambda_j + is}{\lambda_j - is}\right)^{N-1} \left(\frac{\lambda_j - i(s+1)}{\lambda_j + i(s+1)}\right) = \prod_{\substack{k \neq j \\ k=2s+2}}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}\,, j = 2s+2\,, \ldots\,, M\,, \quad (3.25)$$

which follow from the Bethe equations (3.19) with $j = 3, \ldots, M$ after substituting (3.21) and taking $\beta \to 0$.

3.3 XXZ

For the spin-1/2 XXZ spin chain with twisted boundary conditions, the Bethe equations are given by

$$\left(\frac{\sinh(\lambda_j + \frac{\eta}{2})}{\sinh(\lambda_j - \frac{\eta}{2})}\right)^{N} = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^{M} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}\,, \qquad j = 1, \ldots, M\,, \qquad (3.26)$$

where η is the anisotropy parameter, which we assume has a generic value (i.e., $q = e^{\eta}$ is not a root of unity). When $\beta = 0$, these equations have singular solutions of the form

$$\{\frac{\eta}{2}, -\frac{\eta}{2}, \lambda_3, \ldots, \lambda_M\}\,. \qquad (3.27)$$

Repeating the same steps of our argument for the isotropic case, we conclude that a physical singular solution must satisfy the constraint

$$\left[-\prod_{j=3}^{M} \frac{\sinh(\lambda_j + \frac{\eta}{2})}{\sinh(\lambda_j - \frac{\eta}{2})}\right]^{N} = 1\,, \qquad (3.28)$$

as well as

$$\left(\frac{\sinh(\lambda_j + \frac{\eta}{2})}{\sinh(\lambda_j - \frac{\eta}{2})}\right)^{N-1} \frac{\sinh(\lambda_j - \frac{3\eta}{2})}{\sinh(\lambda_j + \frac{3\eta}{2})} = \prod_{\substack{k \neq j \\ k=3}}^{M} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}\,, \; j = 3\,, \cdots, M\,. \tag{3.29}$$

Similarly, for the spin-s XXZ spin chain with twisted boundary conditions, the Bethe equations are given by

$$\left(\frac{\sinh(\lambda_j + s\eta)}{\sinh(\lambda_j - s\eta)}\right)^{N} = e^{-i\beta} \prod_{\substack{k \neq j \\ k=1}}^{M} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}\,, \qquad j = 1, \ldots, M\,. \tag{3.30}$$

When $\beta = 0$, these equations have singular solutions of the form

$$\{s\eta\,, (s-1)\eta\,, \ldots\,, -(s-1)\eta\,, -s\eta\,, \lambda_{2s+2}\,, \ldots\,, \lambda_M\}\,, \tag{3.31}$$

where again all the roots are assumed to be distinct. A physical singular solution of this form must satisfy the constraint

$$\left[(-1)^{2s} \prod_{j=2s+2}^{M} \frac{\sinh(\lambda_j + s\eta)}{\sinh(\lambda_j - s\eta)}\right]^{N} = 1\,, \tag{3.32}$$

as well as

$$\left(\frac{\sinh(\lambda_j + s\eta)}{\sinh(\lambda_j - s\eta)}\right)^{N-1} \frac{\sinh(\lambda_j - (s+1)\eta)}{\sinh(\lambda_j + (s+1)\eta)} = \prod_{\substack{k \neq j \\ k=2s+2}}^{M} \frac{\sinh(\lambda_j - \lambda_k + \eta)}{\sinh(\lambda_j - \lambda_k - \eta)}\,,$$
$$j = 2s+2\,, \ldots\,, M\,. \tag{3.33}$$

The constraint (3.28) and its generalization (3.32), which heretofore had not been written down, can also be straightforwardly derived using the alternative regularization (3.7) following [46] and [56].

3.4 Conclusion

We have argued that a twist regularization can be used to derive the constraints (3.14), (3.24), (3.28), (3.32) for singular solutions of the periodic XXX and XXZ spin chains to be physical. The fact that these constraints can be derived using two different regularizations suggests that they are independent of the choice of regularization. Indeed, the fact that these constraints appear already at first order in the regulator (instead of order N, as suggested by the original derivations [46,56]) implies that they are robust.

Although the arguments presented here demonstrate only that these conditions are necessary, the arguments in [46] and [56] imply that these conditions are also sufficient for singular solutions to be physical. This conclusion is also supported by numerical evidence [47, 56]. The latter references also show that most of the solutions of the Bethe equations are unphysical singular solutions; hence, it is all the more important to have simple criteria for picking out from among the many singular solutions the few that are physical.

As noted in [42, 56], the Bethe equations for chains with $s > 1/2$ can also have singular solutions with repeated roots that are physical. We expect that the twist regularization considered here can also be used to derive conditions for such "strange" singular solutions to be physical.

CHAPTER 4

Boundary energy of the open XXX chain with a non-diagonal boundary term

4.1 Background

Ever since the open spin-1/2 XXX (isotropic) quantum spin chain with non-diagonal boundary terms was shown to be integrable [3, 11, 12], the challenge has been to find its general Bethe ansatz solution. Significant progress has been made recently on this problem. The breakthrough was the realization that the Baxter T-Q equation for this model should have an inhomogeneous term [25] (see also [63]). A simplified version of this solution was subsequently shown to produce all the eigenvalues [30]. A beautiful expression for the corresponding eigenvectors was then proposed in [24]. Another simple solution was found and shown to be complete in [64].

Despite these successes, an important question has remained unanswered: is this solution practical for performing explicit computations in the thermodynamic limit? Due to the inhomogeneous term in the T-Q equation, the corresponding Bethe equations have a non-conventional form; therefore, it appears that conventional Bethe ansatz techniques for analyzing the thermodynamic limit (counting function, root density, etc.) cannot be used.

As a modest step towards addressing this question, we consider here the problem of computing the so-called boundary (or surface) energy of this model. For simplicity, we focus on the limit that the coefficient (ξ) of the non-diagonal boundary term goes to zero, and compute the leading correction (of order ξ^2) to the boundary energy. In this limit, the N Bethe roots for the ground state split evenly into two sets: "small" roots that satisfy the diagonal Bethe equations, and "large" roots that satisfy a generalization of the Richardson-Gaudin equations. The contribution to the leading correction of the boundary energy from each of these sets of roots can be evaluated exactly in the limit $N \to \infty$.

The outline of this paper is as follows. In Section 4.2 we briefly describe the model and recall its Bethe ansatz solution. In Section 4.3 we present the computation of the boundary energy. Our conclusions are presented in Section 4.4.

4.2 The model and its Bethe ansatz solution

We consider the antiferromagnetic open spin-1/2 isotropic quantum spin chain with non-diagonal boundary terms. Following [25], we take as our Hamiltonian

$$H = \sum_{n=1}^{N-1} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} + \frac{1}{q}\,(\sigma_1^z + \xi \sigma_1^x) + \frac{1}{p}\sigma_N^z\,, \tag{4.1}$$

where p, q, ξ are arbitrary real boundary parameters. We consider the solution based on the following linear T-Q equation [30]:

$$\Lambda(\lambda)\,Q(\lambda) = \bar{a}(\lambda)\,Q(\lambda-1) + \bar{d}(\lambda)\,Q(\lambda+1) + 2(1-\sqrt{1+\xi^2})\,(\lambda(\lambda+1))^{2N+1}\,, \tag{4.2}$$

where $\Lambda(\lambda)$ is an eigenvalue of the model's transfer matrix [11, 12, 25]. Moreover,

$$\bar{a}(\lambda) = \frac{2\lambda+2}{2\lambda+1}(\lambda+p)(\sqrt{1+\xi^2}\lambda+q)(\lambda+1)^{2N}\,, \qquad \bar{d}(\lambda) = \bar{a}(-\lambda-1)\,, \tag{4.3}$$

and

$$Q(\lambda) = \prod_{j=1}^{N} (\lambda - \lambda_j)(\lambda + \lambda_j + 1) \,. \tag{4.4}$$

The zeros $\lambda_1, \ldots, \lambda_N$ of $Q(\lambda)$ satisfy the Bethe equations that follow directly from (4.2):

$$\begin{aligned} & e_1(u_j)^{2N}\, e_{2p-1}(u_j)\, e_{2\tilde{q}-1}(u_j) - \prod_{\substack{k \neq j \\ k=1}}^{N} e_2(u_j - u_k)\, e_2(u_j + u_k) \\ & \quad = i\left(1 - \frac{1}{\sqrt{1+\xi^2}}\right) \\ & \quad \times \frac{u_j (u_j + \frac{i}{2})^{2N}}{(u_j - i(p - \frac{1}{2}))(u_j - i(\tilde{q} - \frac{1}{2})) \prod_{\substack{k \neq j \\ k=1}}^{N} (u_j - u_k - i)(u_j + u_k - i)} \,, \\ & \qquad\qquad j = 1, 2, \ldots, N \,, \end{aligned} \tag{4.5}$$

where

$$u_j = i\left(\lambda_j + \tfrac{1}{2}\right) \,, \qquad \tilde{q} = \frac{q}{\sqrt{1+\xi^2}} \,, \qquad e_n(u) = \frac{u + \frac{in}{2}}{u - \frac{in}{2}} \,. \tag{4.6}$$

The eigenvalues of the Hamiltonian (4.1) are given by [30]

$$E = -2 \sum_{j=1}^{N} \frac{1}{u_j^2 + \frac{1}{4}} + N - 1 + \frac{1}{p} + \frac{1}{\tilde{q}} \,. \tag{4.7}$$

We observe that the energy is invariant under $\xi \to -\xi$, since the T-Q equation and Bethe equations have this invariance. Moreover, we can restrict to one sign of q (say, $q > 0$), since the signs of all the boundary terms in the Hamiltonian (4.1) can be changed by a global $SU(2)$ transformation (namely, rotation by π about the y axis, which leaves σ^y invariant, but changes $\sigma^{x,z} \to -\sigma^{x,z}$). For definiteness, we shall further restrict to even values of N, and $p < 0$.

4.3 Boundary energy

For simplicity, we henceforth restrict our attention to the ground state. As is well known, for the corresponding closed chain Hamiltonian with periodic boundary conditions

$$H^{\text{periodic}} = \sum_{n=1}^{N} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} \,, \qquad \vec{\sigma}_{N+1} \equiv \vec{\sigma}_1 \,, \tag{4.8}$$

the ground-state energy $E_0^{\text{periodic}}(N)$ for large N is given by

$$E_0^{\text{periodic}}(N) = N e_\infty + O\left(\tfrac{1}{N}\right) \,, \tag{4.9}$$

where $e_\infty = 1 - 4\ln 2$. In contrast, for the open chain Hamiltonian (4.1), the ground-state energy $E_0(N; p, q, \xi)$ for large N is given by (see, e.g. [14, 15])

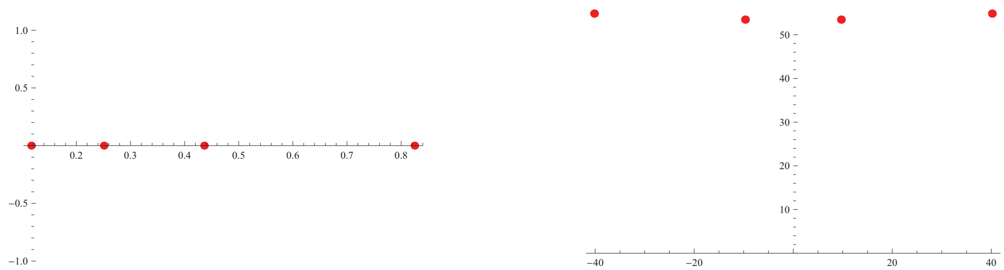
$$E_0(N; p, q, \xi) = N e_\infty + E_b(p, q, \xi) + O\left(\tfrac{1}{N}\right) \,, \tag{4.10}$$

where $E_b(p, q, \xi)$ is the boundary (or surface) energy. Equivalently, we see that the boundary energy is given by

$$E_b(p, q, \xi) = \lim_{N\to\infty} \left[E_0(N; p, q, \xi) - E_0^{\text{periodic}}(N) \right] \,. \tag{4.11}$$

The boundary energy is a function of the boundary parameters, and is arguably the simplest such quantity to compute in the thermodynamic limit. For $\xi = 0$, the boundary terms in the Hamiltonian (4.1) become diagonal, and the exact boundary energy is known [65–68],

$$\begin{aligned} E_b(p, q, \xi = 0) &= \frac{1}{p} + \frac{1}{q} - 1 + \pi - 2\int_0^\infty dx\, \frac{e^{-(2q-1)x} - e^{(2p-1)x} + e^{-x}}{\cosh x} \qquad (4.12) \\ &= \frac{1}{p} + \frac{1}{q} - 1 + \pi - \ln 4 + \psi\left(\tfrac{q}{2}\right) - \psi\left(\tfrac{1+q}{2}\right) + \psi\left(\tfrac{2-p}{2}\right) - \psi\left(\tfrac{1-p}{2}\right) , \end{aligned}$$



(a) (b)

Figure 4.1: The exact small (a) and large (b) Bethe roots for the ground state with $p = -8\,, q = 4\,, \xi = \frac{1}{8}\,, N = 8$.

where $\psi(x)$ is the digamma function, and we have assumed that $q > 0\,, p < 0$.

Unfortunately, the corresponding result for general values of ξ is still out of reach. We therefore consider the series expansion of the boundary energy about $\xi = 0$,

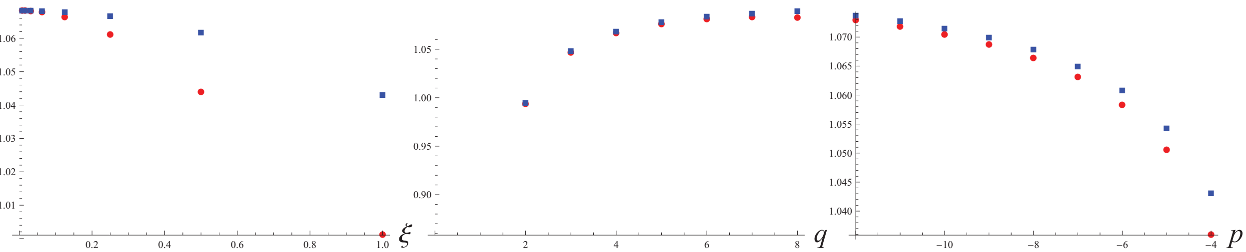
$$E_b(p,q,\xi) = E_b(p,q,\xi=0) + E_b^{(1)}(p,q)\,\xi^2 + O\left(\xi^4\right)\,, \tag{4.13}$$

which contains only even powers of ξ since the energy is invariant under $\xi \to -\xi$. We focus here on computing only the leading correction $E_b^{(1)}(p,q)$.

From numerical studies for small values of N (using the methods in [30]), we find that the N Bethe roots $\{u_1\,, \ldots\,, u_N\}$ describing the ground state split evenly into two sets as $\xi \to 0$: "small" roots $\{v_1\,, \ldots\,, v_{N/2}\}$ that remain finite, and "large" roots $\{w_1\,, \ldots\,, w_{N/2}\}$ that grow as $1/\xi$. An example is shown in Fig. 4.1. We now proceed to consider separately the contributions to $E_b^{(1)}(p,q)$ from these two sets of roots.

4.3.1 Small roots

For large values of N, we assume that the Bethe roots $\{v_1\,, \ldots\,, v_{N/2}\}$ that remain finite as $\xi \to 0$ decouple from the large roots and approximately satisfy the diagonal



(a) (b) (c)

Figure 4.2: The boundary energy from the exact small roots ($E_0^{\rm small}(N) - E_0^{\rm periodic}(N)$) is plotted with red circles; the boundary energy from the roots obtained using the diagonal Bethe equations (4.14) ($E_0^{\rm diag}(N) - E_0^{\rm periodic}(N)$) is plotted with blue squares. In (a), $p = -8\,, q = 4$ and ξ is varied; in (b), $p = -8\,, \xi = \frac{1}{8}$ and q is varied; in (c), $q = 4\,, \xi = \frac{1}{8}$ and p is varied. In all three figures, $N = 8$.

reduction of the exact Bethe equations (**??**), namely,

$$e_1(v_j)^{2N}\, e_{2p-1}(v_j)\, e_{2\tilde{q}-1}(v_j) = \prod_{\substack{k\neq j \\ k=1}}^{\frac{N}{2}} e_2(v_j - v_k)\, e_2(v_j + v_k)\,, \qquad j = 1\,, \ldots\,, \frac{N}{2}\,. \tag{4.14}$$

These roots still depend on ξ through $\tilde{q}$. As a check on this assumption, we have compared (for $N = 8$, and for various values of the boundary parameters) the boundary energy contributions from the exact small roots, and from the Bethe roots obtained using the diagonal Bethe equations (4.14). We find that the agreement is very good for small values of ξ, as shown in Fig. 4.2.

The contribution of these small roots to the boundary energy is given by (4.12) with q replaced by $\tilde{q}$. Expanding this result in powers of ξ, we recover the ξ-independent term $E_b(p, q, \xi = 0)$ in (4.13), and we obtain from the term of order ξ^2 the following contribution to $E_b^{(1)}(p, q)$ from the small roots:

$$E_b^{(1)\,\rm small}(p,q) = \frac{1}{2q} - \frac{q}{4}\left[\psi'\left(\frac{q}{2}\right) - \psi'\left(\frac{q+1}{2}\right)\right]\,. \tag{4.15}$$

4.3.2 Large roots

For the Bethe roots $\{w_1\,, \ldots\,, w_{N/2}\}$ that grow as $1/\xi$ for $\xi \to 0$, we derive an approximate equation by expanding the exact Bethe equations (**??**) to first order in ξ using

$$\frac{a+b}{a-b} = 1 + \frac{2b}{a} + O\left(\left(\frac{b}{a}\right)^2\right)\,, \qquad |a| \gg |b|\,. \tag{4.16}$$

We obtain

$$\begin{aligned}(p+q-1)\frac{1}{w_j} &= \sum_{\substack{k\neq j\\ k=1}}^{\frac{N}{2}}\left(\frac{1}{w_j - w_k} + \frac{1}{w_j + w_k}\right) + \tfrac{1}{4}\xi^2 w_j \prod_{\substack{k\neq j\\ k=1}}^{\frac{N}{2}} \frac{1}{1-\left(\frac{w_k}{w_j}\right)^2}\,,\\ j &= 1\,, \ldots\,, \frac{N}{2}\,.\end{aligned} \tag{4.17}$$

These equations have some resemblance to those appearing in the Richardson-Gaudin models [69, 70]. However, the final term, which is due to the inhomogeneous term in the T-Q equation (4.2), is completely new.

It is hopeless to try to solve this equation directly, especially for large values of N. We proceed by instead recasting it in the form of a T-Q-type equation, which however will be a differential (rather than finite-difference) equation. (Such a strategy has been used for related problems in e.g. [14, 71–74].) To this end, we introduce the polynomial $\mathsf{q}(w)$ of degree N with zeros $\pm w_k$,

$$\mathsf{q}(w) \equiv \prod_{k=1}^{\frac{N}{2}} (w - w_k)(w + w_k)\,, \tag{4.18}$$

which has the asymptotic behavior

$$\mathsf{q}(w) \sim w^N \quad \text{for} \quad w \to \infty\,. \tag{4.19}$$

We observe the identities

$$\frac{\mathsf{q}''(w_j)}{\mathsf{q}'(w_j)} = \frac{1}{w_j} + 2\sum_{k\neq j}\left(\frac{1}{w_j - w_k} + \frac{1}{w_j + w_k}\right) , \tag{4.20}$$

and

$$\mathsf{q}'(w_j) = 2w_j^{N-1}\prod_{k\neq j}\left[1 - \left(\frac{w_k}{w_j}\right)^2\right] , \tag{4.21}$$

where the prime denotes differentiation with respect to w. It follows that (4.17) is equivalent to

$$w_j\mathsf{q}''(w_j) - (2p + 2q - 1)\mathsf{q}'(w_j) + \xi^2 w_j^{N+1} = 0\,, \tag{4.22}$$

The equation obtained by replacing w_j with $-w_j$ in (4.22) is consistent with (4.22), since $\mathsf{q}''(-w_j) = \mathsf{q}''(w_j)\,,\ \mathsf{q}'(-w_j) = -\mathsf{q}'(w_j)$, and N is even. Therefore, the function

$$w\mathsf{q}''(w) - (2p + 2q - 1)\mathsf{q}'(w) + \xi^2 w^{N+1}$$

has all the zeros of $\mathsf{q}(w)$, and is a polynomial of degree $N+1$. It follows that

$$w\mathsf{q}''(w) - (2p + 2q - 1)\mathsf{q}'(w) + \xi^2 w^{N+1} = t(w)\,\mathsf{q}(w)\,, \tag{4.23}$$

where $t(w)$ is a polynomial of degree 1, i.e., $t(w) = t_1 w + t_0$. The asymptotic behavior (4.19) implies that $t_1 = \xi^2\,, t_0 = 0$. We conclude that the zeros of $\mathsf{q}(w)$ (and therefore the solutions of (4.17)) can be determined from the T-Q-type equation

$$w\mathsf{q}''(w) - (2p + 2q - 1)\mathsf{q}'(w) + \xi^2 w^{N+1} - \xi^2 w\mathsf{q}(w) = 0\,. \tag{4.24}$$

Remarkably, the unusual term in the Richardson-Gaudin-type equations (4.17) (that originated from the inhomogeneous term in the T-Q equation (4.2)) has been seamlessly accommodated.

Since the Bethe roots $\{w_j\}$ grow as $1/\xi$ for $\xi \to 0$, it is convenient to introduce rescaled quantities

$$x_j = w_j \xi\,, \qquad x = w\xi\,, \tag{4.25}$$

and the corresponding polynomial

$$g(x) \equiv \prod_{k=1}^{\frac{N}{2}} (x - x_k)(x + x_k)\,. \tag{4.26}$$

Evidently, $\mathsf{q}(w) = \xi^{-N} g(x)$, and therefore (4.24) becomes

$$x \frac{1}{g(x)} \frac{d^2 g(x)}{dx^2} - (2p + 2q - 1) \frac{1}{g(x)} \frac{dg(x)}{dx} + \frac{x^{N+1}}{g(x)} - x = 0\,. \tag{4.27}$$

Note that the ξ dependence has disappeared. This equation (or, equivalently, Eq.(4.24)) can be easily solved numerically for the zeros of $g(x)$ even for large values of N, as shown in the example of Fig. 4.3.

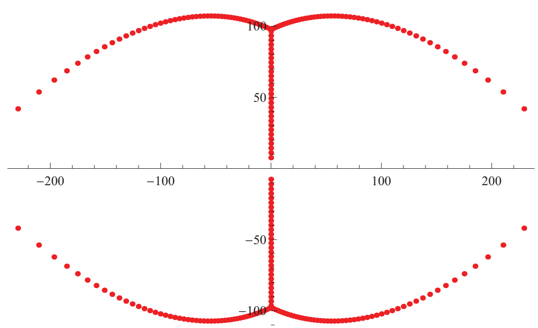


Figure 4.3: The zeros of $g(x)$ for $p = -8\,, q = 4\,, N = 256$.

We observe that the term $\frac{x^{N+1}}{g(x)}$ in (4.27) goes to 0 for $x \sim 0$ and $N \to \infty$. Indeed, $g(x)$ has no zeros near the origin (provided, as we henceforth assume, that $p+q$ is not a positive integer), and therefore the denominator is nonzero, while the numerator approaches zero rapidly for $x < 1$ and $N \to \infty$. Hence, after dropping this term, the rescaled T-Q-type equation (4.27) can be written as

$$x\left(\frac{dG(x)}{dx} + G(x)^2 - 1\right) - (2p+2q-1)G(x) = 0\,, \qquad (x \sim 0)\,, \tag{4.28}$$

where

$$G(x) \equiv \frac{1}{g(x)}\frac{dg(x)}{dx} = \sum_{k=1}^{\frac{N}{2}}\left(\frac{1}{x-x_k} + \frac{1}{x+x_k}\right). \tag{4.29}$$

The contribution of the large roots to the energy (4.7) can be expressed in terms of the derivative of $G(x)$ at $x = 0$:

$$E^{\text{large}} = -2\sum_{j=1}^{\frac{N}{2}}\frac{1}{w_j^2+\frac{1}{4}} \approx -2\xi^2\sum_{j=1}^{\frac{N}{2}}\frac{1}{x_j^2} = \xi^2\left.\frac{dG(x)}{dx}\right|_{x=0}. \tag{4.30}$$

The contribution of the large roots to $E_b^{(1)}(p,q)$ (4.13) is therefore

$$E_b^{(1)\,\text{large}}(p,q) = \left.\frac{dG(x)}{dx}\right|_{x=0}. \tag{4.31}$$

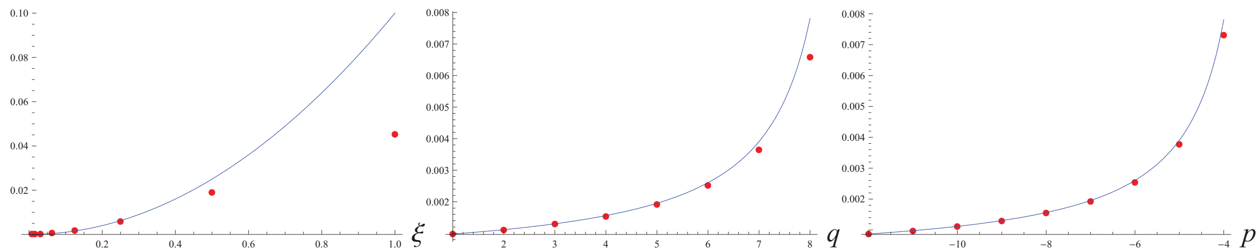
The first-order differential equation (4.28) can be solved in closed form

$$G(x) = -i\frac{J_{p+q-1}(-ix) + CY_{p+q-1}(-ix)}{J_{p+q}(-ix) + CY_{p+q}(-ix)}\,, \tag{4.32}$$

where $J_n(x)$ and $Y_n(x)$ are Bessel functions of the first and second kind, respectively, and C is an arbitrary constant. The requirement that $G(x)$ should be finite at $x = 0$ uniquely determines C, which however depends on the value of $p+q$. For example, if $p+q \le 0$ and $p+q \ne -1/2$, then $C = 0$.

One way to evaluate (4.31) is to expand the Bessel functions in (4.32) about $x = 0$ and obtain the $O(x)$ term. Even easier is to substitute $G(x) = \alpha x + O(x^2)$ into (4.28) and solve for the constant α. We obtain

$$E_b^{(1)\,\text{large}}(p,q) = \frac{1}{2(1-p-q)}\,. \tag{4.33}$$



(a) (b) (c)

Figure 4.4: The energy from the exact large roots ($E_0^{\text{large}}(N)$) for $N = 8$ is plotted with red circles; the $N \to \infty$ result $E_b^{(1)\,\text{large}}(p,q)\,\xi^2$, with $E_b^{(1)\,\text{large}}(p,q)$ given by (4.33), is the blue curve. In (a), $p = -8\,, q = 4$ and ξ is varied; in (b), $p = -8\,, \xi = \frac{1}{8}$ and q is varied; in (c), $q = 4\,, \xi = \frac{1}{8}$ and p is varied.

In deriving the result (4.33) for the contribution from the large roots to the boundary energy, we have assumed that $N \to \infty$. Surprisingly, this result is accurate even for small values of N (provided that ξ is small), as shown for $N = 8$ in Fig. 4.4.

4.3.3 Final result

Adding the results from the small roots (4.15) and the large roots (4.33), we obtain our final result for the leading correction to the boundary energy (defined in Eq. (4.13))

$$\begin{aligned} E_b^{(1)}(p,q) &= E_b^{(1)\,\text{small}}(p,q) + E_b^{(1)\,\text{large}}(p,q) \\ &= \frac{1}{2q} - \frac{q}{4}\left[\psi'\left(\frac{q}{2}\right) - \psi'\left(\frac{q+1}{2}\right)\right] + \frac{1}{2(1-p-q)}\,. \end{aligned} \tag{4.34}$$

We have already noted in Figs. 4.2 and 4.4 some partial checks using numerical results for $N = 8$. In principle, the final result (4.34) could be checked by comparing with numerical results for sufficiently large values of N. Indeed, boundary energies were estimated for the $\xi = 0$ case in [15] using extrapolation with values of N up to 256. However, we have not (yet) managed to accurately solve the exact Bethe equations (**??**) numerically for the ground state Bethe roots with such large values of N.

4.4 Conclusion

We have argued that the recently-found Bethe ansatz solution [25,30] of the model (4.1) can be used to perform a computation in the thermodynamic limit. Indeed, at least for small values of ξ, the inhomogeneous term in the T-Q equation (4.2), which leads to an unusual term in the Richardson-Gaudin-type equations (4.17) for the large roots, does not impede the derivation of an analytical expression (4.34) for the boundary energy. It would be interesting if one could pass directly from the T-Q equation (4.2) to the T-Q-type equation (4.24), without first going through the equations (4.17).

There are many interesting related problems: computing higher-order corrections in ξ and finite-size ($1/N$) corrections to the ground-state energy, considering excited states, etc. However, such computations may require developing additional techniques.

4.5 Erratum

We emphasized that our computation of the boundary energy relies on several assumptions (in particular, the decoupling of the "small" and "large" roots), and that the result should therefore be checked numerically. Although we have not managed to solve the Bethe equations numerically for sufficiently large values of N, we have succeeded to use the Density Matrix Renormalization Group (DMRG) method, as implemented by the Algorithms and Libraries for Physics Simulations (ALPS) [75], to compute the ground-state energy of the open chain up to 256 sites. Sample results are presented in Table 4.1. Following [15], the large-N extrapolation of the boundary energy was performed using the van den Broeck-Schwartz algorithm [76–78] from the sequence $N = 4, 6, 8, \ldots, 60$. Note that $e_\infty = 1 - 4\ln 2$.

N	$E_0(N)$	$E_0(N) - Ne_\infty$
4	-6.50010714011	0.5902477488
8	-13.5365249173	0.6441848606
16	-27.6843594238	0.6770601320
32	-56.0271138616	0.6957252501
64	-112.739844063	0.7058341603
128	-226.180208854	0.7111475927
256	-453.068824003	0.7138888904
∞		0.7167

Table 4.1: Ground-state energy and boundary energy of the open chain with boundary parameters $p = -8\,, q = 4\,, \xi = \frac{1}{8}$.

The extrapolated result for the boundary energy, $E_b = 0.7167$, is consistent with the contribution attributed to only the "small" roots,

$$E_b(p, q, \xi = 0) + E_b^{(1)\,\mathrm{small}}\,\xi^2\,, \tag{4.35}$$

where $E_b(p, q, \xi = 0)$ and $E_b^{(1)\,\mathrm{small}}$ are given by (4.12) and (4.15) , respectively. Indeed, evaluating (4.35) for our choice of boundary parameters gives 0.716711, while adding the contribution from the "large" roots

$$\frac{1}{2(1-p-q)}\xi^2 \tag{4.36}$$

would yield a too-high value (0.718273) for the boundary energy.

This result suggests that the boundary energy should be given entirely by (4.35) up to order ξ^2, and therefore by

$$E_b = \frac{1}{p} + \frac{1}{\tilde{q}} - 1 + \pi - 2\int_0^\infty dx\, \frac{e^{-(2\tilde{q}-1)x} - e^{(2p-1)x} + e^{-x}}{\cosh x}\,, \qquad \tilde{q} = \frac{q}{\sqrt{1+\xi^2}}\,, \tag{4.37}$$

for general values of ξ. Another argument for dropping the contribution (4.36) is that it remains constant in the limit $q \to \infty$ and $p \to -\infty$ with $p + q$ constant, which is inconsistent with the fact that the Hamiltonian becomes independent of ξ in this limit. Moreover, (4.35) and (4.37) can be resolved into a sum of separate contributions from the two boundaries, as naively expected. The result (4.37) has recently been derived by other means [79], see also [64].

The source of error in our computation is likely to be the assumption of decoupling of the "small" and "large" roots. Unfortunately, it is not clear how to directly compute the contribution to the boundary energy due to the coupling of these two types of roots, which presumably should cancel (4.36).

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CHAPTER 5

Quantum group symmetries and completeness for $A_{2n}^{(2)}$ open spin chains

5.1 Background

Interesting new connections of integrable quantum spin chains to integrable quantum field theory, conformal field theory (CFT) and string theory, as well as to condensed matter physics, continue to be found. A case in point concerns the $A_n^{(2)}$ family of models [80–83], which has recently been revisited by Vernier *et al.* [84–86]. For example, it was argued in [84] that the $A_2^{(2)}$ model [80] has a regime where the continuum limit is a certain non-compact CFT, the so-called black hole sigma model [87, 88].

Another interesting feature of these models is that they can have quantum group symmetries (see e.g. [89, 90]), provided that the boundary conditions are suitable. For the closed chains with periodic boundary conditions studied in [84–86], such symmetries can be realized only indirectly; however, quantum group symmetries can be realized directly in open chains [91].

Motivated in part by these recent developments, we have set out to revisit the quantum group symmetries of the $A_n^{(2)}$ family of models. We therefore focus instead on *open* chains; and, for concreteness, we restrict here to the even series $A^{(2)}_{2n}$, leaving the odd series $A^{(2)}_{2n-1}$ for a future publication. It has long been known that, for one simple set of integrable boundary conditions, the former models have $U_q(B_n)$ symmetry [23, 92].

We argue here that – surprisingly – the $A^{(2)}_{2n}$ models have $U_q(C_n)$ symmetry for another set of integrable boundary conditions. (The symmetry for the case $n = 1$ was already noticed in [31], but the symmetry for the general case $n > 1$ had remained unexplored until now.) This deformation of C_n is novel, with a nonstandard coproduct (5.77). The symmetries (both $U_q(B_n)$ and $U_q(C_n)$) determine the degeneracies and multiplicities of the spectra, which are completely described by the Bethe ansatz solutions.

The outline of this paper is as follows. In Section 5.2 we briefly review the construction of the integrable $A^{(2)}_{2n}$ open quantum spin chains that are the focus of this paper. In Section 5.3 we show that the Hamiltonians for the two cases of interest can be expressed as sums of two-body terms. We use this fact in Section 5.4 to demonstrate that the Hamiltonians have quantum group symmetries, which in turn determine the degeneracies and multiplicities of the spectra. In Section 5.5 we briefly review the Bethe ansatz solutions of the models, and we obtain a formula for the Dynkin labels of the Bethe states, part of whose proof is sketched in an appendix. In Section 5.6 we use this formula to help verify numerically that the Bethe ansatz solutions completely account for the degeneracies and multiplicities implied by the quantum group symmetries. In Section 5.7 we briefly summarize our conclusions, and list some interesting open problems.

5.2 The models

We briefly review here the construction of the integrable $A_{2n}^{(2)}$ open quantum spin chains that will turn out to have quantum group symmetries. The basic ingredients are the R-matrix and K-matrices, which are used to construct a commuting transfer matrix that contains the integrable Hamiltonian.

5.2.1 R-matrix

The R-matrix is a matrix-valued function $R(u)$ of the so-called spectral parameter u that maps $\mathcal{V} \otimes \mathcal{V}$ to itself, where here $\mathcal{V}$ is a $(2n+1)$-dimensional vector space, which is a solution of the Yang-Baxter equation (YBE) on $\mathcal{V} \otimes \mathcal{V} \otimes \mathcal{V}$

$$R_{12}(u-v)\, R_{13}(u)\, R_{23}(v) = R_{23}(v)\, R_{13}(u)\, R_{12}(u-v)\,. \tag{5.1}$$

We use the standard notations $R_{12} = R \otimes \mathbb{I}\,, R_{23} = \mathbb{I} \otimes R\,, R_{13} = \mathcal{P}_{23} R_{12} \mathcal{P}_{23}$, where $\mathbb{I}$ is the identity matrix on $\mathcal{V}$, and $\mathcal{P}$ is the permutation matrix on $\mathcal{V} \otimes \mathcal{V}$

$$\mathcal{P} = \sum_{\alpha,\beta=1}^{2n+1} e_{\alpha\beta} \otimes e_{\beta\alpha}\,, \tag{5.2}$$

and $e_{\alpha\beta}$ are the $(2n+1) \times (2n+1)$ elementary matrices with elements $(e_{\alpha\beta})_{ij} = \delta_{\alpha,i}\delta_{\beta,j}$.

We focus here on the R-matrix (5.115) that is associated with the fundamental representation of $A_{2n}^{(2)}$ [81–83] with anisotropy parameter η, which is a generalization of the Izergin-Korepin R-matrix [80] that is associated with $A_2^{(2)}$. Besides satisfying the YBE, this R-matrix enjoys several additional important properties, among them PT symmetry

$$R_{21}(u) \equiv \mathcal{P}_{12}\, R_{12}(u)\, \mathcal{P}_{12} = R_{12}^{t_1 t_2}(u)\,, \tag{5.3}$$

unitarity

$$R_{12}(u)\ R_{21}(-u) = \xi(u)\, \xi(-u)\, \mathbb{I} \otimes \mathbb{I}\,, \tag{5.4}$$

where $\xi(u)$ is given by

$$\xi(u) = 2\sinh(\frac{u}{2} - 2\eta) \cosh(\frac{u}{2} - (2n+1)\eta)\,, \tag{5.5}$$

regularity

$$R(0) = \xi(0)\, \mathcal{P}\,, \tag{5.6}$$

and crossing symmetry

$$R_{12}(u) = V_1\, R_{12}^{t_2}(-u-\rho)\, V_1 = V_2^{t_2}\, R_{12}^{t_1}(-u-\rho)\, V_2^{t_2}\,, \tag{5.7}$$

where $\rho = -i\pi - 2(2n+1)\eta$; and the matrix V, which is given by (5.119), satisfies $V^2 = \mathbb{I}$.

5.2.2 K-matrices

The matrix $K^-(u)$, which maps $\mathcal{V}$ to itself, is a solution of the boundary Yang-Baxter equation (BYBE) on $\mathcal{V} \otimes \mathcal{V}$ [3, 10, 11, 22]

$$R_{12}(u-v)\, K_1^-(u)\ R_{21}(u+v)\, K_2^-(v) = K_2^-(v)\, R_{12}(u+v)\, K_1^-(u)\, R_{21}(u-v)\,. \tag{5.8}$$

The matrix $K^-(u)$ is assumed to have the regularity property

$$K^-(0) = \kappa\, \mathbb{I}\,. \tag{5.9}$$

Similarly, $K^+(u)$ satisfies [11, 22]

$$\begin{aligned} &R_{12}(-u+v)\, K_1^{+\,t_1}(u)\, M_1^{-1}\, R_{21}(-u-v-2\rho)\, M_1\, K_2^{+\,t_2}(v) \\ &\quad = K_2^{+\,t_2}(v)\, M_1\, R_{12}(-u-v-2\rho)\, M_1^{-1}\, K_1^{+\,t_1}(u)\, R_{21}(-u+v)\,, \end{aligned} \tag{5.10}$$

where the matrix M is defined by

$$M = V^t\, V\,, \tag{5.11}$$

and is given by (5.120). If $K^-(u)$ is a solution of the BYBE (5.8), then [11, 22]

$$K^+(u) = K^{-\,t}(-u-\rho)\, M \tag{5.12}$$

is a solution of (5.10).

We consider here two different sets of K-matrices:

$$(I): \qquad K^-(u) = \mathbb{I}\,, \qquad K^+(u) = M\,, \tag{5.13}$$

$$(II): \qquad K^-(u) = K(u)\,, \quad K^+(u) = K(-u-\rho)\, M\,. \tag{5.14}$$

The fact that $K^-(u) = \mathbb{I}$ is a solution of the BYBE was noted in [23]. The matrix $K(u)$ in (5.14) is the diagonal matrix given by

$$K(u) = \mathrm{diag}(k_1(u), \ldots, k_{2n+1}(u))\,, \tag{5.15}$$

where

$$k_j(u) = \begin{cases} e^{-u}\left[\epsilon i \cosh\eta + \sinh(u - 2n\eta)\right] & j = 1, \ldots, n \\ \epsilon i \cosh(u+\eta) - \sinh(2n\eta) & j = n+1 \\ e^{u}\left[\epsilon i \cosh\eta + \sinh(u - 2n\eta)\right] & j = n+2, \ldots, 2n+1 \end{cases}\,, \tag{5.16}$$

where ϵ can have the values ± 1, but for concreteness we henceforth set $\epsilon = +1$. This K-matrix has the regularity property (5.9) with

$$\kappa = i \cosh\eta - \sinh(2n\eta)\,. \tag{5.17}$$

The solution (5.15)-(5.16) of the BYBE (5.8) for the case $n = 1$ was found in [23], and the generalization for $n > 1$ was found in [93, 94].

5.2.3 Transfer matrix and Hamiltonian

The transfer matrix $t(u)$ for an integrable open quantum spin chain with N sites, which acts on the quantum space $\mathcal{V}^{\otimes N}$, is given by [11]

$$t(u) = \mathrm{tr}_a\, K^+_a(u)\, T_a(u)\, K^-_a(u)\, \hat{T}_a(u)\,, \tag{5.18}$$

where the monodromy matrices are defined by

$$T_a(u) = R_{aN}(u)\ R_{aN-1}(u)\ \cdots R_{a1}(u)\,, \hat{T}_a(u) = R_{1a}(u)\ \cdots R_{N-1a}(u)\ R_{Na}(u)\,, \tag{5.19}$$

and the trace in (5.18) is over the auxiliary space, which we denote by a. The various properties satisfied by the R and K matrices can be used to show that the transfer matrix satisfies the fundamental commutativity property [11]

$$[t(u)\,, t(v)] = 0 \text{ for all } u\,, v\,. \tag{5.20}$$

The corresponding integrable open chain Hamiltonian $\mathcal{H}$ is given (up to multiplicative and additive constants) by $t'(0)$, which evidently satisfies

$$[\mathcal{H}\,, t(u)] = 0\,. \tag{5.21}$$

More explicitly, one finds [11]

$$\mathcal{H} = \sum_{k=1}^{N-1} h_{k,k+1} + \frac{1}{2\kappa} {K^-_1}'(0) + \frac{1}{\mathrm{tr}\, K^+(0)}\, \mathrm{tr}_0\, K^+_0(0) h_{N0}\,, \tag{5.22}$$

where the two-site Hamiltonian $h_{k,k+1}$ is given by

$$h_{k,k+1} = \frac{1}{\xi(0)} \mathcal{P}_{k,k+1} R'_{k,k+1}(0)\,. \tag{5.23}$$

5.3 Simplification of the Hamiltonian

We show here that the boundary terms in the Hamiltonian (5.22) can be simplified for the two sets of K-matrices (5.13), (5.14) in such a way that the Hamiltonians are expressed as sums of two-body terms, which will allow us to demonstrate their quantum group invariance in the following section. The key step in this simplification is a K-matrix identity (5.24), which is reminiscent of Sklyanin's "less obvious" isomorphism given by Eqs. (17) and (18) in [11], and the Ghoshal-Zamolodchikov boundary crossing-unitarity relation, see Eqs. (3.33) and (3.35) in [3].

5.3.1 An identity for the K-matrix

A useful identity is

$$\mathrm{tr}_1\, K_1^{-}(-u-\rho)\, M_1\, R_{12}(2u)\, \mathcal{P}_{12} = f(u)\, V_2\, K_2^{-\,t_2}(u)\, V_2\,, \tag{5.24}$$

where $f(u)$ is a scalar function. The remainder of this subsection is devoted to proving this identity. Readers who are more interested to see how this identity can be used to simplify the boundary terms in the Hamiltonian may skip directly to Sec. 5.3.2.

It is helpful to recall (see e.g. [29]) that the crossing symmetry (5.7) can be used to show that the R-matrix degenerates at $u = -\rho$ to a projector onto a one-dimensional subspace,

$$\tilde{P}_{12}^{-} \equiv \frac{1}{(2n+1)\,\xi(0)} R_{12}(-\rho) = \frac{1}{(2n+1)} V_1\, \mathcal{P}_{12}^{t_2}\, V_1\,, \tag{5.25}$$

which obeys

$$\left(\tilde{P}_{12}^{-}\right)^2 = \tilde{P}_{12}^{-} \tag{5.26}$$

and

$$\tilde{P}^-_{12}\, A_{12}\, \tilde{P}^-_{12} = \mathrm{tr}_{12}\left(\tilde{P}^-_{12} A_{12}\right) \tilde{P}^-_{12}\,, \tag{5.27}$$

where A is an arbitrary matrix acting on $\mathcal{V} \otimes \mathcal{V}$. This projector is not symmetric,

$$\tilde{P}^-_{21} \equiv \mathcal{P}_{12}\, \tilde{P}^-_{12}\, \mathcal{P}_{12} = (\tilde{P}^-_{12})^{t_1 t_2} \neq \tilde{P}^-_{12}\,. \tag{5.28}$$

We also recall that

$$V_1\, R_{12}(u)\, V_1 = V_2\, R_{21}(u)\, V_2\,. \tag{5.29}$$

The starting point of the proof is the BYBE (5.8), where we set $v = -u - \rho$ and use the definition (5.25) to obtain

$$R_{12}(2u+\rho)\, K^-_1(u)\, \tilde{P}^-_{21}\, K^-_2(-u-\rho) = K^-_2(-u-\rho)\, \tilde{P}^-_{12}\, K^-_1(u)\, R_{21}(2u+\rho)\,. \tag{5.30}$$

With the help of the relations

$$\tilde{P}^-_{21} = V_1^{t_1}\, V_2^{t_2}\, \tilde{P}^-_{12}\, V_1^{t_1}\, V_2^{t_2} \tag{5.31}$$

and

$$R_{21}(2u+\rho) = V_1^{t_1}\, V_2^{t_2}\, R_{12}(2u+\rho)\, V_1^{t_1}\, V_2^{t_2} \tag{5.32}$$

that follow from (5.29), we arrive at

$$\begin{aligned} &R_{12}(2u+\rho)\, K^-_1(u)\, V_1^{t_1}\, V_2^{t_2}\, \tilde{P}^-_{12}\, V_2^{t_2}\, K^-_2(-u-\rho) \\ &\quad = K^-_2(-u-\rho)\, \tilde{P}^-_{12}\, K^-_1(u)\, V_1^{t_1}\, V_2^{t_2}\, R_{12}(2u+\rho)\, V_2^{t_2}\,. \end{aligned} \tag{5.33}$$

Multiplying both sides on the right by $\tilde{P}^-_{12}$ and using the projector property (5.27), we obtain

$$R_{12}(2u+\rho)\, K^-_1(u)\, V_1^{t_1}\, V_2^{t_2}\, \tilde{P}^-_{12} = g(u)\, K^-_2(-u-\rho)\, \tilde{P}^-_{12}\,, \tag{5.34}$$

where $g(u)$ is some scalar function. Multiplying both sides, on both the right and the left, by the permutation matrix $\mathcal{P}_{12}$, and then using the crossing equation (5.7) and the expression (5.25) for $\tilde{P}^{-}_{12}$, we obtain

$$V_1^{t_1}\, R_{12}^{t_1}(-2u-2\rho)\, K_2^{-}(u)\, V_1^{t_1}\, V_2^{t_2}\, \mathcal{P}_{12}^{t_1}\, V_1^{t_1} = g(u)\, K_1^{-}(-u-\rho)\, V_1^{t_1}\, \mathcal{P}_{12}^{t_1}\, V_1^{t_1}\,, \tag{5.35}$$

Taking the trace of both sides over the first space, we arrive at

$$\mathrm{tr}_1\, R_{12}^{t_1}(-2u-2\rho)\, K_2^{-}(u)\, V_1^{t_1}\, V_2^{t_2}\, \mathcal{P}_{12}^{t_1} = g(u)\ \mathrm{tr}_1\, K_1^{-}(-u-\rho)\, V_1^{t_1}\, \mathcal{P}_{12}^{t_1}\, V_1^{t_1}\,, \tag{5.36}$$

which can be simplified to

$$\mathrm{tr}_1\, K_1^{-}(u)\, M_1\, R_{12}(-2u-2\rho)\, \mathcal{P}_{12} = g(u)\, V_2\, K_2^{-\,t_2}(-u-\rho)\, V_2\,. \tag{5.37}$$

Replacing $u \mapsto -u-\rho$ and setting $f(u) = g(-u-\rho)$, we finally obtain (5.24).

5.3.2 Simplified Hamiltonians

We now proceed to simplify the boundary terms in the Hamiltonian (5.22) using the identity (5.24), which can be rewritten as

$$\mathrm{tr}_1\, K_1^{+}(u)\, \mathcal{P}_{12} R_{21}(2u) = f(u)\, V_2\, K_2^{-}(u)\, V_2 \tag{5.38}$$

for diagonal $K^{\pm}$-matrices that are related by (5.12).

5.3.2.1 Set I

For the first set of K-matrices (5.13), the identity (5.38) immediately implies that

$$\mathrm{tr}_1\, M_1\, \mathcal{P}_{12} R_{21}(2u) = f(u)\, \mathbb{I}_2\,. \tag{5.39}$$

Differentiating this relation with respect to u and then setting $u = 0$, we obtain the result

$$\mathrm{tr}_1\, M_1\, \mathcal{P}_{12} R'_{21}(0) \propto \mathbb{I}_2 \tag{5.40}$$

(see also [23, 95]) and therefore

$$\mathrm{tr}_0\, K_0^+(0) h_{N0} = \mathrm{tr}_0\, M_0 h_{N0} \propto \mathrm{tr}_0\, M_0 \mathcal{P}_{N0} R'_{N0}(0) \propto \mathbb{I}_N\,, \tag{5.41}$$

i.e. the corresponding boundary term is proportional to the identity matrix. Moreover, since $K^-(u) = \mathbb{I}$, the boundary term with $K^{-\prime}(0)$ evidently vanishes.

In short, the two boundary terms in the expression (5.22) for the Hamiltonian can be dropped. The Hamiltonian for the set I therefore reduces to a sum of two-site Hamiltonians [23]

$$\mathcal{H}^{(I)} = \sum_{k=1}^{N-1} h_{k,k+1}\,. \tag{5.42}$$

Its relation to the transfer matrix (5.18) is given by

$$\mathcal{H}^{(I)} = \frac{1}{c_1} t'(0) + c_2 \mathbb{I}^{\otimes N}\,, \tag{5.43}$$

with

$$\begin{aligned} c_1 &= 4^{N+1} \sinh((2n+1)\eta)\, \cosh((2n-1)\eta)\, \sinh^{2N-1}(2\eta)\, \cosh^{2N}((2n+1)\eta)\,, \\ c_2 &= \frac{\cosh((6n+1)\eta)}{2\sinh((4n+2)\eta)\, \cosh((2n-1)\eta)}\,. \end{aligned} \tag{5.44}$$

5.3.2.2 Set II

We turn now to the second set of K-matrices (5.14). Setting $u = 0$ in the identity (5.38), and using the regularity properties (5.6) and (5.9), we obtain

$$f(0) = \frac{1}{\kappa}\, \xi(0)\, \mathrm{tr}\, K^+(0)\,. \tag{5.45}$$

Moreover, differentiating the identity (5.38) with respect to u and then setting $u = 0$, we obtain

$$2\,\mathrm{tr}_1\, K_1^+(0)\,\mathcal{P}_{12} R_{21}'(0) + \ldots = f(0)\, V_2\, K_2^{-\,\prime}(0) V_2\; + \ldots\,, \tag{5.46}$$

where the ellipses represent terms that are proportional to the identity, which we drop. Using the explicit form of the K-matrix (5.15)-(5.16), we observe that

$$V\, K^{-\,\prime}(0)\, V = -K^{-\,\prime}(0) + \mu U + \nu \mathbb{I}\,, \tag{5.47}$$

where

$$\mu = 2(i\sinh\eta - \cosh(2n\eta))\,, \qquad \nu = 2\cosh(2n\eta)\,, \qquad U = e_{n+1,n+1}\,. \tag{5.48}$$

Substituting (5.45) and (5.47) into (5.46), we arrive at the identity

$$\frac{1}{\xi(0)\ \mathrm{tr}\, K^+(0)}\, \mathrm{tr}_1\, K_1^+(0)\,\mathcal{P}_{12} R_{21}'(0) = -\frac{1}{2\kappa} K_2^{-\,\prime}(0) + \frac{\mu}{2\kappa} U_2 + \ldots \tag{5.49}$$

The Hamiltonian (5.22) for the set II therefore reduces to the form

$$\mathcal{H}^{(II)} = \sum_{k=1}^{N-1} h_{k,k+1} + \frac{1}{2\kappa}\left[K_1^{-\,\prime}(0) - K_N^{-\,\prime}(0)\right] + \frac{\mu}{2\kappa} U_N\,. \tag{5.50}$$

Let us define a new two-site Hamiltonian $\tilde{h}_{k,k+1}$ as follows

$$\tilde{h}_{k,k+1} \equiv h_{k,k+1} + \frac{1}{2\kappa}\left[K_k'(0) - K_{k+1}'(0)\right]\,. \tag{5.51}$$

We conclude that, up to a term proportional to U_N, the Hamiltonian again reduces to a sum of two-site Hamiltonians,

$$\mathcal{H}^{(II)} = \sum_{k=1}^{N-1} \tilde{h}_{k,k+1} + \frac{\mu}{2\kappa} U_N\,. \tag{5.52}$$

Its relation to the transfer matrix (5.18) is given by

$$\mathcal{H}^{(II)} = \frac{1}{c_1} t'(0) + c_2 \mathbb{I}^{\otimes N} \,, \tag{5.53}$$

with

$$\begin{aligned} c_1 &= 2^{2N+1} (\cosh\eta + i\sinh(2n\eta))^2 \, \sinh((4n+2)\eta)\cosh((2n+3)\eta) \\ &\quad \times [\sinh(2\eta)\, \cosh((2n+1)\eta)]^{2N-1} \,, \\ c_2 &= \frac{\cosh((6n+5)\eta)}{2\sinh((4n+2)\eta)\, \cosh((2n+3)\eta)} + \frac{i\cosh(2n\eta)}{\cosh\eta + i\sinh(2n\eta)} \,. \end{aligned} \tag{5.54}$$

5.4 Quantum group symmetries

We first review the $U_q(B_n)$ symmetry of the Hamiltonian corresponding to the first set of K-matrices (5.13). We then argue that the Hamiltonian corresponding to the second set of K-matrices (5.14) has the quantum group symmetry $U_q(C_n)$.

5.4.1 Set I: $U_q(B_n)$ symmetry

It was already argued in [23] that the Hamiltonian $\mathcal{H}^{(I)}$ (5.42) corresponding to the first set of K-matrices (5.13) has $U_q(B_n)$ symmetry. It was subsequently shown in [92] (generalizing the arguments in [96] for the XXZ chain) that this symmetry extends to the full transfer matrix $t(u)$ (5.18). Here we explicitly construct the coproduct of the generators, and show that they commute with the Hamiltonian.

For the vector representation of $B_n = O(2n+1)$, in the so-called *orthogonal* basis, the Cartan generators $\{H_1, \ldots, H_n\}$ are given by the diagonal matrices [1]

$$H_\alpha = e_{\alpha,\alpha} - e_{2n+2-\alpha,2n+2-\alpha} \,, \qquad \alpha = 1, 2, \ldots, n \,, \tag{5.55}$$

[1]Explicit matrix representations for the generators can be obtained from e.g. [97] or Maple.

and the generators $\{E_1^\pm, \ldots, E_n^\pm\}$ corresponding to the simple roots are given by

$$E_\alpha^+ = e_{\alpha,\alpha+1} + e_{2n+1-\alpha,2n+2-\alpha}\,, \qquad E_\alpha^- = E_\alpha^{+\,t}\,, \qquad \alpha = 1, 2, \ldots, n\,. \tag{5.56}$$

Indeed, these generators satisfy

$$\left[H_i\,, E_j^\pm\right] = \pm\alpha_i^{(j)} E_j^\pm\,, \qquad i, j = 1, 2, \ldots, n\,, \tag{5.57}$$

where $\{\alpha^{(1)}, \ldots, \alpha^{(n)}\}$ are the simple roots of B_n in the orthogonal basis (see e.g. [98])

$$\begin{aligned} \alpha^{(1)} &= (1, -1, 0, \ldots, 0)\,, \\ \alpha^{(2)} &= (0, 1, -1, 0, \ldots, 0)\,, \\ &\vdots \\ \alpha^{(n-1)} &= (0, \ldots, 0, 1, -1)\,, \\ \alpha^{(n)} &= (0, \ldots, 0, 1)\,. \end{aligned} \tag{5.58}$$

Let us define the following coproduct for these generators

$$\begin{aligned} \Delta(H_j) &= H_j \otimes \mathbb{I} + \mathbb{I} \otimes H_j\,, \\ \Delta(E_j^\pm) &= E_j^\pm \otimes e^{i\pi H_j} e^{\eta(H_j - H_{j+1})} + e^{-i\pi H_j} e^{-\eta(H_j - H_{j+1})} \otimes E_j^\pm\,, \end{aligned} \tag{5.59}$$

where $j = 1, \ldots, n$ with $H_{n+1} \equiv 0$. We observe that

$$\Omega_{ij}\,\Delta(E_i^+)\,\Delta(E_j^-) - \Delta(E_j^-)\,\Delta(E_i^+)\,\Omega_{ij} = \delta_{i,j}\frac{q^{\Delta(H_i)-\Delta(H_{i+1})} - q^{-\Delta(H_i)+\Delta(H_{i+1})}}{q - q^{-1}}\,, \tag{5.60}$$

where $q = e^{2\eta}$ and

$$\Omega_{ij} = \begin{cases} e^{i\pi H_{\max(i,j)}} \otimes \mathbb{I} & |i-j| = 1 \\ \mathbb{I} \otimes \mathbb{I} & |i-j| \neq 1 \end{cases}\,. \tag{5.61}$$

The two-site Hamiltonian (5.23) commutes with the coproducts (5.59)

$$\left[\Delta(H_j)\,, h_{1,2}\right] = \left[\Delta(E_j^{\pm})\,, h_{1,2}\right] = 0\,, \qquad j = 1, \ldots, n\,. \tag{5.62}$$

Since the N-site Hamiltonian is given (5.42) by the sum of two-site Hamiltonians, it follows that the N-site Hamiltonian commutes with the N-fold coproducts

$$\left[\Delta_{(N)}(H_j)\,, \mathcal{H}^{(I)}\right] = \left[\Delta_{(N)}(E_j^{\pm})\,, \mathcal{H}^{(I)}\right] = 0\,, \qquad j = 1, \ldots, n\,. \tag{5.63}$$

This provides an explicit demonstration of the $U_q(B_n)$ invariance of the Hamiltonian $\mathcal{H}^{(I)}$.

5.4.1.1 Degeneracies and multiplicities for $U_q(B_n)$

One of the important consequences of the $U_q(B_n)$ symmetry of the Hamiltonian is that the energy eigenstates form irreducible representations of this algebra. For generic values of η (i.e., $\eta \neq i\pi/p$, where p is a rational number), the representations are the same as for the classical algebra B_n. The generalization of the familiar Clebsch-Gordan theorem from $A_1 = SU(2)$ to B_n implies that the N-site Hilbert space has a decomposition of the form

$$\mathcal{V}^{(2n+1)\otimes N} = \bigoplus_j d^{(j,N,n)}\, \mathcal{V}^{(j)}\,, \tag{5.64}$$

where $\mathcal{V}^{(j)}$ denotes an irreducible representation of B_n with dimension j (= degeneracy of the corresponding energy eigenvalue) and $d^{(j,N,n)}$ is its multiplicity. Here we specify the irreducible representations by their dimensions, and we allow for the possibility that there can be more than one inequivalent irreducible representation with a given dimension. For example, B_2 has a **35** and a **35′**.

The first few cases are as follows (see e.g. [98]): [2]

$$
\begin{aligned}
B_1: \qquad N &= 2: \qquad \mathbf{3}\otimes\mathbf{3} = \mathbf{1}\oplus\mathbf{3}\oplus\mathbf{5} \\
&\qquad\qquad = [0]\oplus[2]\oplus[4] \\
N &= 3: \qquad \mathbf{3}\otimes\mathbf{3}\otimes\mathbf{3} = \mathbf{1}\oplus 3\cdot\mathbf{3}\oplus 2\cdot\mathbf{5}\oplus\mathbf{7} \\
&\qquad\qquad = [0]\oplus 3[2]\oplus 2[4]\oplus[6]
\end{aligned} \tag{5.65}
$$

$$
\begin{aligned}
B_2: \qquad N &= 2: \qquad \mathbf{5}\otimes\mathbf{5} = \mathbf{1}\oplus\mathbf{10}\oplus\mathbf{14} \\
&\qquad\qquad = [0,0]\oplus[0,2]\oplus[2,0] \\
N &= 3: \qquad \mathbf{5}\otimes\mathbf{5}\otimes\mathbf{5} = 3\cdot\mathbf{5}\oplus\mathbf{10}\oplus\mathbf{30}\oplus 2\cdot\mathbf{35} \\
&\qquad\qquad = 3[1,0]\oplus[0,2]\oplus[3,0]\oplus 2[1,2]
\end{aligned} \tag{5.66}
$$

$$
\begin{aligned}
B_3: \qquad N &= 2: \qquad \mathbf{7}\otimes\mathbf{7} = \mathbf{1}\oplus\mathbf{21}\oplus\mathbf{27} \\
&\qquad\qquad = [0,0,0]\oplus[0,1,0]\oplus[2,0,0] \\
N &= 3: \qquad \mathbf{7}\otimes\mathbf{7}\otimes\mathbf{7} = 3\cdot\mathbf{7}\oplus\mathbf{35}\oplus\mathbf{77}\oplus 2\cdot\mathbf{105} \\
&\qquad\qquad = 3[1,0,0]\oplus[0,0,2]\oplus[3,0,0]\oplus 2[1,1,0]
\end{aligned} \tag{5.67}
$$

We have verified numerically that the Hamiltonian as well as the transfer matrix for set I (5.13) have exactly these degeneracies and multiplicities for generic values of η, which provides further evidence of their $U_q(B_n)$ invariance.

[2] For later reference, we also present the tensor-product decompositions in terms of the Dynkin labels $[a_1, \ldots, a_n]$ of the representations.

5.4.2 Set II: $U_q(C_n)$ symmetry

For the vector representation of $C_n = Sp(2n)$ in the orthogonal basis, the Cartan generators are given by

$$\tilde{H}_\alpha = \tilde{e}_{\alpha,\alpha} - \tilde{e}_{2n+1-\alpha,2n+1-\alpha}\,, \qquad \alpha = 1, 2, \ldots, n\,, \tag{5.68}$$

and the generators corresponding to the simple roots are given by

$$\begin{aligned} \tilde{E}^+_\alpha &= \tilde{e}_{\alpha,\alpha+1} + \tilde{e}_{2n-\alpha,2n+1-\alpha}\,, \qquad \alpha = 1, 2, \ldots, n-1\,, \\ \tilde{E}^+_n &= \tilde{e}_{n,n+1}\,, \end{aligned} \tag{5.69}$$

and $\tilde{E}^-_\alpha = \tilde{E}^{+\,t}_\alpha$, where $\tilde{e}_{\alpha\beta}$ are the elementary $(2n)\times(2n)$ matrices. These generators satisfy

$$\left[\tilde{H}_i\,, \tilde{E}^\pm_j\right] = \pm\alpha^{(j)}_i\,\tilde{E}^\pm_j\,, \qquad i, j = 1, 2, \ldots, n\,, \tag{5.70}$$

where $\{\alpha^{(1)}, \ldots, \alpha^{(n)}\}$ are the simple roots of C_n in the orthogonal basis

$$\begin{aligned} \alpha^{(1)} &= (1, -1, 0, \ldots, 0)\,, \\ \alpha^{(2)} &= (0, 1, -1, 0, \ldots, 0)\,, \\ &\vdots \\ \alpha^{(n-1)} &= (0, \ldots, 0, 1, -1)\,, \\ \alpha^{(n)} &= (0, \ldots, 0, 2)\,, \end{aligned} \tag{5.71}$$

c.f. (5.58).

Let us now consider the Hamiltonian $\mathcal{H}^{(II)}$ (5.52) corresponding to the second set of K-matrices (5.14). The appearance of $U_q(C_n)$ symmetry in this spin chain can be understood as a sort of "breaking" of B_n down to C_n. That is, we consider an embedding of C_n in B_n, such that the vector space $\mathcal{V}^{(2n+1)}$ at each site, which forms a $(2n+1)$-dimensional irreducible representation of B_n, decomposes into the direct sum of the $2n$-dimensional and 1-dimensional irreducible representations of C_n,

$$\mathcal{V}^{(2n+1)} = \mathcal{W}^{(2n)} \oplus \mathcal{W}^{(1)} . \tag{5.72}$$

We construct the corresponding generators of C_n on $\mathcal{V}^{(2n+1)}$ by starting from the vector representation of the C_n generators in terms of $(2n) \times (2n)$ matrices (5.68)-(5.69), and then inserting a column of 0's between columns n and $n+1$, and a row of 0's between rows n and $n+1$, thereby arriving at a set of $(2n+1) \times (2n+1)$ matrices. That is,

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \mapsto \begin{pmatrix} A & 0 & B \\ 0 & 0 & 0 \\ C & 0 & D \end{pmatrix} , \tag{5.73}$$

where A, B, C, D represent $n \times n$ matrices.

In short, we henceforth represent the generators of C_n by $(2n+1) \times (2n+1)$ matrices, such that the Cartan generators are given by the diagonal matrices

$$H_\alpha = e_{\alpha,\alpha} - e_{2n+2-\alpha,2n+2-\alpha} \,, \qquad \alpha = 1, 2, \ldots, n \,, \tag{5.74}$$

and the generators corresponding to the simple roots are given by

$$\begin{aligned} E_\alpha^+ &= e_{\alpha,\alpha+1} + e_{2n+1-\alpha,2n+2-\alpha} \,, \qquad \alpha = 1, 2, \ldots, n-1 \,, \\ E_n^+ &= e_{n,n+2} \,, \end{aligned} \tag{5.75}$$

and $E_\alpha^- = E_\alpha^{+\,t}$. Comparing with the corresponding expressions for the generators of B_n (5.55)-(5.56), we see that they are exactly the same, except for $E_n^\pm$.

We propose the following coproduct for these generators

$$\Delta(H_j) = H_j \otimes \mathbb{I} + \mathbb{I} \otimes H_j \,, \qquad j = 1, \ldots, n \,, \tag{5.76}$$

and

$$\begin{aligned}
\Delta(E_j^{\pm}) &= E_j^{\pm} \otimes e^{i\pi H_{j+1}} + e^{i\pi H_{j+1}} e^{-2\eta(H_j - H_{j+1})} \otimes E_j^{\pm} \,, \qquad j = 1, \ldots, n-1 \,, \\
\Delta(E_n^{\pm}) &= E_n^{\pm} \otimes \mathbb{I} + e^{4\eta H_n} \otimes E_n^{\pm} \\
&\pm \sinh(2\eta) \Big\{ e^{i\pi H_{n-1}} \left[E_n^{\pm} \,, E_{n-1}^{\pm} \right] \otimes e^{i\pi H_n} E_{n-1}^{\mp} \\
&\quad - e^{4\eta H_n} e^{i\pi H_n} E_{n-1}^{\mp} \otimes e^{-4\eta H_{n-1}} e^{i\pi H_{n-1}} \left[E_n^{\pm} \,, E_{n-1}^{\pm} \right] \\
&\quad - e^{-\eta(H_n - H_{n-2})} \left[\left[E_n^{\pm} \,, E_{n-1}^{\pm} \right] \,, E_{n-2}^{\pm} \right] \otimes e^{-\eta(H_n + H_{n-2})} \left[E_{n-1}^{\mp} \,, E_{n-2}^{\mp} \right] \\
&\quad + e^{3\eta(H_n + H_{n-2})} \left[E_{n-1}^{\mp} \,, E_{n-2}^{\mp} \right] \otimes e^{3\eta(H_n - H_{n-2})} \left[\left[E_n^{\pm} \,, E_{n-1}^{\pm} \right] \,, E_{n-2}^{\pm} \right] + \ldots \Big\} \,,
\end{aligned} \tag{5.77}$$

c.f. (5.59). The result for $\Delta(E_n^{\pm})$ is particularly unusual; the ellipsis represents additional contributions involving higher nested commutators, whose precise form for $n > 3$ remains to be worked out. The series terminates with terms involving an $(n-1)$-fold nested commutator. We observe the following relations for $1 \le i, j < n$:

$$\begin{aligned}
\Delta(E_i^{+})\, \Delta(E_i^{-}) - e^{4\eta}\, \Delta(E_i^{-})\, \Delta(E_i^{+}) &= \frac{e^{-4\eta(\Delta(H_i) - \Delta(H_{i+1}))} - \mathbb{I} \otimes \mathbb{I}}{e^{-4\eta} - 1} \,, \\
e^{2\eta}\, \Omega_{ij}\, \Delta(E_i^{+})\, \Delta(E_j^{-}) &= \Delta(E_j^{-})\, \Delta(E_i^{+})\, \Omega_{ij} \,, \quad |i-j| = 1 \\
\Delta(E_i^{+})\, \Delta(E_j^{-}) &= \Delta(E_j^{-})\, \Delta(E_i^{+}) \,, \quad |i-j| \ge 2 \,,
\end{aligned} \tag{5.78}$$

where Ω_{ij} is given by (5.61). Moreover,

$$\Delta(E_n^+)\,\Delta(E_n^-) - e^{-8\eta}\,\Delta(E_n^-)\,\Delta(E_n^+) = \frac{e^{8\eta\Delta(H_n)} - \mathbb{I}\otimes\mathbb{I}}{e^{8\eta}-1} +$$

$$+e^{-4\eta}\sinh^2(2\eta)\left\{\left(\sum_{k=1}^{n-1} H_k^2 + \left[\sum_{k=1}^{n-1}\cosh(4\eta k)\right] e^{4\eta H_n} H_n^2\right)\otimes e^{4\eta H_n} H_n\right.$$

$$\left. + e^{4\eta H_n} H_n \otimes \left(\sum_{k=1}^{n-1} H_k^2 + \left[\sum_{k=1}^{n-1}\cosh(4\eta k)\right] e^{4\eta H_n} H_n^2\right)\right\}. \quad (5.79)$$

We conjecture the following deformed Serre relations

$$\sum_{k=0}^{1-a_{ij}} (-1)^k c_{ijk} \Delta(E_i^+)^{1-a_{ij}-k}\,\Delta(E_j^+)\,\Delta(E_i^+)^k = 0\,, \qquad i = 1,\ldots,n\,, \qquad j > i\,, \quad (5.80)$$

where $a_{ij} = 2\alpha^{(i)}\cdot\alpha^{(j)}/\alpha^{(i)}\cdot\alpha^{(i)}$, and the coefficients c_{ijk} satisfy

$$c_{i,j,1} = \begin{cases} -2\cosh(2\eta)\, c_{i,i+1,0} & i+1 = j < n \\ c_{i,j,0} & i+1 < j \le n \end{cases},$$

$$c_{i,i+1,2} = \begin{cases} c_{i,i+1,0} & i < n-1 \\ e^{4\eta} c_{n-1,n,1} & i = n-1 \end{cases}, \quad (5.81)$$

and similar relations for $\Delta(E_i^-)$. The relations (5.76)-(5.81) (which we have fully checked only up to $n=3$) define, in part, a deformation of C_n, which evidently reduces to the classical algebra for $\eta \to 0$. It would be interesting to further understand this realization of $U_q(C_n)$.

By construction, the coproducts (5.76)-(5.77) commute with the "new" two-site Hamiltonian (5.51)

$$\left[\Delta(H_j)\,,\tilde{h}_{1,2}\right] = \left[\Delta(E_j^\pm)\,,\tilde{h}_{1,2}\right] = 0\,, \qquad j = 1,\ldots,n\,. \quad (5.82)$$

Moreover, all the generators (whose row $(n+1)$ and column $(n+1)$ are null, as in (5.73)) evidently commute with $U = e_{n+1,n+1}$. Since the N-site Hamiltonian is given (5.52) by the sum of two-site Hamiltonians and a term proportional to U_N, it follows that the N-site Hamiltonian commutes with the N-fold coproducts

$$\left[\Delta_{(N)}(H_j)\,, \mathcal{H}^{(II)}\right] = \left[\Delta_{(N)}(E_j^{\pm})\,, \mathcal{H}^{(II)}\right] = 0\,, \qquad j = 1, \ldots, n\,, \tag{5.83}$$

which implies the $U_q(C_n)$ invariance of the Hamiltonian $\mathcal{H}^{(II)}$. We conjecture that this symmetry also extends to the full transfer matrix. The symmetry for the case $n = 1$ (note that $C_1 = A_1$) was first noted in [31].

5.4.2.1 Degeneracies and multiplicities for $U_q(C_n)$

The $U_q(C_n)$ invariance of the Hamiltonian implies that, for generic values of η, the N-site Hilbert space has a decomposition of the form (cf. Eq. (5.64))

$$\left(\mathcal{W}^{(2n)} \oplus \mathcal{W}^{(1)}\right)^{\otimes N} = \bigoplus_j \tilde{d}^{(j,N,n)}\, \mathcal{W}^{(j)}\,, \tag{5.84}$$

where $\mathcal{W}^{(j)}$ denotes an irreducible representation of C_n with dimension j (= degeneracy of the corresponding energy eigenvalue) and $\tilde{d}^{(j,N,n)}$ is its multiplicity.

The first few cases are as follows (see again e.g. [98]):

$$\begin{aligned}
C_1 = A_1: \qquad N &= 2: \qquad (\mathbf{2} \oplus \mathbf{1})^{\otimes 2} = 2 \cdot \mathbf{1} \oplus 2 \cdot \mathbf{2} \oplus \mathbf{3} \\
&\qquad\qquad\qquad\quad = 2[0] \oplus 2[1] \oplus [2] \\
N &= 3: \qquad (\mathbf{2} \oplus \mathbf{1})^{\otimes 3} = 4 \cdot \mathbf{1} \oplus 5 \cdot \mathbf{2} \oplus 3 \cdot \mathbf{3} \oplus \mathbf{4} \\
&\qquad\qquad\qquad\quad = 4[0] \oplus 5[1] \oplus 3[2] \oplus [3]
\end{aligned} \tag{5.85}$$

$$
\begin{aligned}
C_2: \qquad N &= 2: \qquad (\mathbf{4} \oplus \mathbf{1})^{\otimes 2} = 2 \cdot \mathbf{1} \oplus 2 \cdot \mathbf{4} \oplus \mathbf{5} \oplus \mathbf{10} \\
&\qquad\qquad = 2[0,0] \oplus 2[1,0] \oplus [0,1] \oplus [2,0] \\
N &= 3: \qquad (\mathbf{4} \oplus \mathbf{1})^{\otimes 3} = 4 \cdot \mathbf{1} \oplus 6 \cdot \mathbf{4} \oplus 3 \cdot \mathbf{5} \oplus 3 \cdot \mathbf{10} \oplus 2 \cdot \mathbf{16} \oplus \mathbf{20} \\
&\qquad\qquad = 4[0,0] \oplus 6[1,0] \oplus 3[0,1] \oplus 3[2,0] \oplus 2[1,1] \oplus [3,0]
\end{aligned}
\tag{5.86}
$$

$$
\begin{aligned}
C_3: \qquad N &= 2: \qquad (\mathbf{6} \oplus \mathbf{1})^{\otimes 2} = 2 \cdot \mathbf{1} \oplus 2 \cdot \mathbf{6} \oplus \mathbf{14} \oplus \mathbf{21} \\
&\qquad\qquad = 2[0,0,0] \oplus 2[1,0,0] \oplus [0,1,0] \oplus [2,0,0] \\
N &= 3: \qquad (\mathbf{6} \oplus \mathbf{1})^{\otimes 3} = 4 \cdot \mathbf{1} \oplus 6 \cdot \mathbf{6} \oplus 3 \cdot \mathbf{14} \oplus \mathbf{14'} \oplus 3 \cdot \mathbf{21} \oplus \mathbf{56} \oplus 2 \cdot \mathbf{64} \\
&\qquad\qquad = 4[0,0,0] \oplus 6[1,0,0] \oplus 3[0,1,0] \oplus [0,0,1] \oplus \\
&\qquad\qquad\quad \oplus 3[2,0,0] \oplus [3,0,0] \oplus 2[1,1,0]
\end{aligned}
\tag{5.87}
$$

We have verified numerically that the Hamiltonian as well as the transfer matrix for set II (5.14) have exactly these degeneracies and multiplicities for generic values of η, which provides further evidence of their $U_q(C_n)$ invariance.

5.5 Bethe ansatz

Our discussion so far has not made use of the integrability of the models. However, this integrability has been exploited to obtain Bethe ansatz solutions of the models corresponding to sets I (5.13) and II (5.14) in [99] and [100], respectively. [3]

Here we study how the quantum group symmetry of these models is reflected in their Bethe ansatz solutions. Our main result is a formula for the Dynkin label $(a_1, \ldots, a_n)$ of a Bethe state in terms of the cardinalities $(m_1, \ldots, m_n)$ of the corresponding Bethe roots (i.e., m_i is the number of Bethe roots of type i, where $i = 1, \ldots, n$), see Eq. (5.106). The Dynkin label uniquely characterizes an irreducible representation, and in particular determines its dimension, which is the degeneracy of the corresponding eigenvalue. The number of distinct solutions of the Bethe equations with $(m_1, \ldots, m_n)$ Bethe roots determines the multiplicity. We shall then verify numerically in Sec. 5.6 that, in this way, the patterns of degeneracies and multiplicities predicted by the quantum group symmetry (5.65)-(5.67) and (5.85)-(5.87) are completely accounted for by the Bethe ansatz solutions.

[3] The solution of the $A_{2n}^{(2)}$ family of integrable quantum spin chains has a long history. The initial work was for *closed* chains with periodic boundary conditions. The case $n = 1$ (corresponding to the Izergin-Korepin model [80]) was first solved using the analytical Bethe ansatz approach [17, 18], which gave the eigenvalues (but not the eigenvectors) of the transfer matrix. This approach was subsequently extended to $n > 1$ in [19]. The algebraic Bethe ansatz for the case $n = 1$, which gave also the eigenvectors of the transfer matrix, was formulated in the important work [101]. The seminal work of Sklyanin [11] made it possible to generalize these results to *open* $A_{2n}^{(2)}$ chains. The case $n = 1$ with the first set of K-matrices (5.13) was solved using the analytical Bethe ansatz approach in [102], and this approach was subsequently extended to $n > 1$ in [99]. The algebraic Bethe ansatz for the case $n = 1$ was developed in [103, 104]. Finally, the algebraic Bethe ansatz for $n > 1$ with general diagonal K-matrices [93, 94] was formulated in [100]. An analytical Bethe ansatz approach for the case $n = 1$ with general non-diagonal K-matrices has recently been formulated in [105]. Other related work includes [106–113] .

5.5.1 Review of the Bethe ansatz solutions

Before presenting our formula for the Dynkin labels, we briefly summarize here the Bethe ansatz solutions of the models. The Bethe states, which we denote by

$$|\Lambda^{(m_1,\ldots,m_n)}\rangle = |\{u_1^{(1)},\ldots,u_{m_1}^{(1)}\},\ldots,\{u_1^{(n)},\ldots,u_{m_n}^{(n)}\}\rangle\,, \tag{5.88}$$

depend on n sets of Bethe roots $\{u_1^{(1)},\ldots,u_{m_1}^{(1)}\},\ldots,\{u_1^{(n)},\ldots,u_{m_n}^{(n)}\}$, which are solutions of the following n sets of Bethe equations [99, 100]

$$\begin{aligned}
e_1^{2N}(u_k^{(1)}) &= \prod_{j=1,\, j\neq k}^{m_1} e_2(u_k^{(1)}-u_j^{(1)})\, e_2(u_k^{(1)}+u_j^{(1)}) \prod_{j=1}^{m_2} e_{-1}(u_k^{(1)}-u_j^{(2)}) \\
&\qquad e_{-1}(u_k^{(1)}+u_j^{(2)})\,, \qquad\qquad k=1,\ldots,m_1\,, \\
1 &= \prod_{j=1}^{m_{l-1}} e_{-1}(u_k^{(l)}-u_j^{(l-1)})\, e_{-1}(u_k^{(l)}+u_j^{(l-1)}) \prod_{j=1,\, j\neq k}^{m_l} e_2(u_k^{(l)}-u_j^{(l)})\, e_2(u_k^{(l)}+u_j^{(l)}) \\
&\times \prod_{j=1}^{m_{l+1}} e_{-1}(u_k^{(l)}-u_j^{(l+1)})\, e_{-1}(u_k^{(l)}+u_j^{(l+1)})\,, \quad k=1,\ldots,m_l\,, \quad l=2,\ldots,n-1\,, \\
\chi(u_k^{(n)}) &= \prod_{j=1}^{m_{n-1}} e_{-1}(u_k^{(n)}-u_j^{(n-1)})\, e_{-1}(u_k^{(n)}+u_j^{(n-1)}) \times \prod_{j=1,\, j\neq k}^{m_n} e_2(u_k^{(n)}-u_j^{(n)}) \\
& e_2(u_k^{(n)}+u_j^{(n)})\, e_{-1}(u_k^{(n)}-u_j^{(n)}+i\pi)\, e_{-1}(u_k^{(n)}+u_j^{(n)}+i\pi) \qquad k=1,\ldots,m_n\,,
\end{aligned} \tag{5.89}$$

where here we use the compact notation

$$e_n(u) = \frac{\sinh(\frac{u}{2}+\eta\, n)}{\sinh(\frac{u}{2}-\eta\, n)}\,, \tag{5.90}$$

and

$$\chi(u) = \begin{cases} 1 & \text{for } B_n \\ \left(\frac{\sinh(\frac{1}{2}(u+\eta-\frac{i\pi}{2}))}{\sinh(\frac{1}{2}(u-\eta+\frac{i\pi}{2}))}\right)^2 & \text{for } C_n \end{cases}\,. \tag{5.91}$$

The above equations are for $n > 1$. For $n = 1$, the Bethe equations are given by

$$
\begin{aligned}
e_1^{2N}(u_k^{(1)})\,\chi(u_k^{(1)}) &= \prod_{j=1,\, j\neq k}^{m_1} e_2(u_k^{(1)} - u_j^{(1)})\, e_{-1}(u_k^{(1)} - u_j^{(1)} + i\pi) \\
&\qquad \times e_2(u_k^{(1)} + u_j^{(1)})\, e_{-1}(u_k^{(1)} + u_j^{(1)} + i\pi)\,, \\
k = 1, \ldots, m_1\,. & \qquad (5.92)
\end{aligned}
$$

The Bethe states are certain simultaneous eigenstates of the transfer matrix $t(u)$ (5.18) and the Cartan generators $\Delta_{(N)}(H_i)$ (5.55), (5.59), (5.74), (5.76),

$$
\begin{aligned}
t(u)\,|\Lambda^{(m_1,\ldots,m_n)}\rangle &= \Lambda^{(m_1,\ldots,m_n)}(u)\,|\Lambda^{(m_1,\ldots,m_n)}\rangle\,, \\
\Delta_{(N)}(H_i)\,|\Lambda^{(m_1,\ldots,m_n)}\rangle &= h_i\,|\Lambda^{(m_1,\ldots,m_n)}\rangle\,, \qquad i = 1, \ldots, n\,. \qquad (5.93)
\end{aligned}
$$

The eigenvalues of the transfer matrix are given by [99, 100]

$$
\begin{aligned}
&\Lambda^{(m_1\,,\cdots\,,m_n)}(u) \\
&= A^{(m_1)}(u)\,\psi_1(u)\ \frac{\sinh(u-2(2n+1)\eta)}{\sinh(u-2\eta)} \\
&\frac{\cosh(u-(2n-1)\eta)}{\cosh(u-(2n+1)\eta)}\left[2\sinh(\frac{u}{2}-2\eta)\cosh(\frac{u}{2}-(2n+1)\eta)\right]^{2N} \\
&+C^{(m_1)}(u)\,\tilde{\psi}_1(u)\ \frac{\sinh u}{\sinh(u-4n\eta)}\frac{\cosh(u-(2n+3)\eta)}{\cosh(u-(2n+1)\eta)} \\
&\left[2\sinh(\frac{u}{2})\cosh(\frac{u}{2}-(2n-1)\eta)\right]^{2N} \\
&+\{w(u)\,\psi_2(u)\,B_n^{(m_n)}(u) + \sum_{l=1}^{n-1}[z_l(u)\,\psi_1(u)\,B_l^{(m_l\,,m_{l+1})}(u) \\
&+\tilde{z}_l(u)\,\tilde{\psi}_1(u)\,\tilde{B}_l^{(m_l\,,m_{l+1})}(u)]\} \times \left[2\sinh(\frac{u}{2})\cosh(\frac{u}{2}-(2n+1)\eta)\right]^{2N}\,, \qquad (5.94)
\end{aligned}
$$

where

$$
A^{(m_1)}(u) = \prod_{j=1}^{m_1}\frac{\sinh(\frac{1}{2}(u-u_j^{(1)})+\eta)\ \sinh(\frac{1}{2}(u+u_j^{(1)})+\eta)}{\sinh(\frac{1}{2}(u-u_j^{(1)})-\eta)\ \sinh(\frac{1}{2}(u+u_j^{(1)})-\eta)}\,, \qquad (5.95)
$$

$$\begin{aligned} C^{(m_1)}(u) &= A^{(m_1)}(-u-\rho) \\ &= \prod_{j=1}^{m_1} \frac{\cosh(\frac{1}{2}(u-u_j^{(1)})-2(n+1)\eta)\ \cosh(\frac{1}{2}(u+u_j^{(1)})-2(n+1)\eta)}{\cosh(\frac{1}{2}(u-u_j^{(1)})-2n\eta)\ \cosh(\frac{1}{2}(u+u_j^{(1)})-2n\eta)}\,, \end{aligned} \tag{5.96}$$

$$\begin{aligned} B_l^{(m_l\,,m_{l+1})}(u) &= \prod_{j=1}^{m_l} \frac{\sinh(\frac{1}{2}(u-u_j^{(l)})-(l+2)\eta)\ \sinh(\frac{1}{2}(u+u_j^{(l)})-(l+2)\eta)}{\sinh(\frac{1}{2}(u-u_j^{(l)})-l\eta)\ \sinh(\frac{1}{2}(u+u_j^{(l)})-l\eta)} \\ &\times \prod_{j=1}^{m_{l+1}} \frac{\sinh(\frac{1}{2}(u-u_j^{(l+1)})-(l-1)\eta)\ \sinh(\frac{1}{2}(u+u_j^{(l+1)})-(l-1)\eta)}{\sinh(\frac{1}{2}(u-u_j^{(l+1)})-(l+1)\eta)\ \sinh(\frac{1}{2}(u+u_j^{(l+1)})-(l+1)\eta)} \\ \tilde{B}_l^{(m_l\,,m_{l+1})}(u) &= B_l^{(m_l\,,m_{l+1})}(-u-\rho)\,, \qquad l=1\,,\cdots\,,n-1\,, \end{aligned} \tag{5.97}$$

$$\begin{aligned} B_n^{(m_n)}(u) &= \prod_{j=1}^{m_n} \frac{\sinh(\frac{1}{2}(u-u_j^{(n)})-(n+2)\eta)\ \sinh(\frac{1}{2}(u+u_j^{(n)})-(n+2)\eta)}{\sinh(\frac{1}{2}(u-u_j^{(n)})-n\eta)\ \sinh(\frac{1}{2}(u+u_j^{(n)})-n\eta)} \\ &\times \frac{\cosh(\frac{1}{2}(u-u_j^{(n)})-(n-1)\eta)\ \cosh(\frac{1}{2}(u+u_j^{(n)})-(n-1)\eta)}{\cosh(\frac{1}{2}(u-u_j^{(n)})-(n+1)\eta)\ \cosh(\frac{1}{2}(u+u_j^{(n)})-(n+1)\eta)}\,, \end{aligned} \tag{5.98}$$

and

$$\begin{aligned} z_l(u) &= \frac{\sinh(u)}{\sinh(u-2l\eta)} \frac{\sinh(u-2(2n+1)\eta)}{\sinh(u-2(l+1)\eta)} \frac{\cosh(u-(2n-1)\eta)}{\cosh(u-(2n+1)\eta)}\,, \\ \tilde{z}_l(u) &= z_l(-u-\rho)\,, \qquad\qquad l=1\,,\cdots\,,n-1\,, \\ w(u) &= \frac{\sinh(u)}{\sinh(u-2n\eta)} \frac{\sinh(u-2(2n+1)\eta)}{\sinh(u-2(n+1)\eta)}\,, \end{aligned} \tag{5.99}$$

where

$$\begin{aligned} \psi_1(u) &= \begin{cases} 1 & \text{for } B_n \\ \frac{\cosh(u-(2n+3)\eta)}{\cosh(u-(2n-1)\eta)}\left[\cosh\eta - i\sinh(u-2n\eta)\right]^2 & \text{for } C_n \end{cases}\,, \\ \tilde{\psi}_1(u) &= \psi_1(-u-\rho)\,, \\ \psi_2(u) &= \begin{cases} 1 & \text{for } B_n \\ \cosh(u-(2n+3)\eta)\ \cosh(u-(2n-1)\eta) & \text{for } C_n \end{cases}\,. \end{aligned} \tag{5.100}$$

The eigenvalues of both Hamiltonians $\mathcal{H}^{(I)}$ and $\mathcal{H}^{(II)}$ are given by

$$E = -\sum_{k=1}^{m_1} \frac{\sinh(2\eta)}{2\sinh(\frac{1}{2}u_k^{(1)} - \eta)\sinh(\frac{1}{2}u_k^{(1)} + \eta)} - \frac{(N-1)\cosh((2n+3)\eta)}{2\sinh(2\eta)\,\cosh((2n+1)\eta)}\,, \tag{5.101}$$

as follows from (5.43)-(5.44), (5.53)-(5.54), and (5.94)-(5.100).

The Bethe states have been constructed in [100] using the nested algebraic Bethe ansatz approach. The "double-row" monodromy matrix

$$\mathcal{T}_a(u) = T_a(u)\, K_a^-(u)\, \hat{T}_a(u) \tag{5.102}$$

can be written as a $(2n+1)\times(2n+1)$ matrix in the auxiliary space whose matrix elements are operators on the quantum space $\mathcal{V}^{\otimes N}$

$$\mathcal{T}_a(u) = \begin{pmatrix} A_1(u) & B_2(u) & B_3(u) & \ldots & B_{2n}(u) & F(u) \\ * & * & * & \ldots & * & * \\ \vdots & \vdots & \vdots & \ldots & \vdots & \vdots \\ * & * & * & \ldots & * & * \\ G(u) & C_2(u) & C_3(u) & \ldots & C_{2n}(u) & A_{2n+1}(u) \end{pmatrix}_{(2n+1)\times(2n+1)} . \tag{5.103}$$

The basic idea is to construct the Bethe states using the $B_i(u)$ operators (as well as others) as creation operators acting on the reference state

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{2n+1}^{\otimes N} . \tag{5.104}$$

We conjecture that the (on-shell) Bethe states are highest-weight states of the quantum group

$$\Delta_{(N)}(E_i^+)\,|\Lambda^{(m_1,\ldots,m_n)}\rangle = 0\,, \qquad i = 1, \ldots, n\,, \tag{5.105}$$

as is the case for other integrable open quantum spin chains with quantum group symmetry (see e.g. [91, 92, 99, 102, 114–118]). However, a proof of this conjecture is beyond the scope of this paper. As a consequence of (5.105), degenerate eigenvectors (i.e., linearly independent eigenvectors of the transfer matrix $t(u)$ whose corresponding eigenvalues coincide with the eigenvalue $\Lambda^{(m_1,\ldots,m_n)}(u)$ of the Bethe state $|\Lambda^{(m_1,\ldots,m_n)}\rangle$) which are obtained by acting on the Bethe state with the lowering operators $\Delta_{(N)}(E_i^-)$ form an irreducible representation of the algebra that is uniquely characterized by the (highest) weights of the Bethe state, known as the Dynkin label.

5.5.2 Dynkin labels of the Bethe states

We propose that the Dynkin label $(a_1, \ldots, a_n)$ corresponding to a Bethe state $|\Lambda^{(m_1,\ldots,m_n)}\rangle$ whose Bethe roots have cardinalities $(m_1, \ldots, m_n)$ is given for $n > 1$ by

$$\begin{aligned} a_1 &= N - 2m_1 + m_2 \,, \\ a_i &= m_{i-1} - 2m_i + m_{i+1} \,, \qquad i = 2, \ldots, n-1 \,, \\ a_n &= \begin{cases} 2(m_{n-1} - m_n) & \text{for } B_n \\ m_{n-1} - m_n & \text{for } C_n \end{cases} \,. \end{aligned} \tag{5.106}$$

For $n = 1$,

$$a_1 = \begin{cases} 2(N - m_1) & \text{for } B_1 \\ N - m_1 & \text{for } C_1 \end{cases} \,. \tag{5.107}$$

It is convenient to divide the proof of this result into two parts. The first part of the proof is the relation of the eigenvalues $(h_1, \ldots, h_n)$ of the Cartan generators to the cardinalities $(m_1, \ldots, m_n)$ of the Bethe roots

$$\begin{aligned} h_1 &= N - m_1 \,, \\ h_i &= m_{i-1} - m_i \,, \qquad i = 2, 3, \ldots, n \,. \end{aligned} \tag{5.108}$$

This relation, which was proposed in [99], is the same as for the closed $A_{2n}^{(2)}$ chain [19]. Its proof is sketched in Appendix 5.9.

The second part of the proof is the relation of the Dynkin label $(a_1, \ldots, a_n)$ to the eigenvalues $(h_1, \ldots, h_n)$ of the Cartan generators

$$\begin{aligned} a_i &= h_i - h_{i+1} \,, \qquad i = 1, 2, \ldots, n-1 \,, \\ a_n &= \begin{cases} 2h_n & \text{for } B_n \\ h_n & \text{for } C_n \end{cases} \,. \end{aligned} \tag{5.109}$$

This relation originates from the definition of Dynkin label (see e.g. [98])

$$(h_1, \ldots, h_n) = \sum_{j=1}^{n} a_j \, \omega_j \,, \tag{5.110}$$

where ω_j are the fundamental weights. In the orthogonal basis in which we work (recall Eqs. (5.58), (5.71)), the fundamental weights are given by

$$\begin{aligned} \omega_1 &= (1, 0, 0, 0, \ldots, 0) \,, \\ \omega_2 &= (1, 1, 0, 0, \ldots, 0) \,, \\ \omega_3 &= (1, 1, 1, 0, \ldots, 0) \,, \\ &\vdots \\ \omega_{n-1} &= (1, 1, 1, \ldots, 1, 0) \,, \\ \omega_n &= \begin{cases} (\frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2}) & \text{for } B_n \\ (1, 1, \ldots, 1) & \text{for } C_n \end{cases} \,. \end{aligned} \tag{5.111}$$

Substituting these expressions for the fundamental weights into (5.110), we see that

$$\begin{aligned} h_1 &= a_1 + \ldots + a_{n-1} + \varepsilon\, a_n\,, \\ h_2 &= a_2 + \ldots + a_{n-1} + \varepsilon\, a_n\,, \\ &\vdots \\ h_n &= \varepsilon\, a_n\,, \end{aligned} \tag{5.112}$$

where

$$\varepsilon = \begin{cases} \frac{1}{2} & \text{for } B_n \\ 1 & \text{for } C_n \end{cases} . \tag{5.113}$$

Inverting the relations (5.112), we arrive at the desired result (5.109).

The main result (5.106), (5.107) follows immediately from the two relations (5.108) and (5.109).

Since the Dynkin labels are nonnegative $a_i \ge 0$, the result (5.106) can be inverted to deduce the values of $(m_1, \ldots, m_n)$ for which solutions of the Bethe equations (5.89) with a given value of N can be expected.

5.6 Numerical check of completeness

We present solutions $(\{u_1^{(1)}, \ldots, u_{m_1}^{(1)}\}, \ldots, \{u_1^{(n)}, \ldots, u_{m_n}^{(n)}\})$ of the $A_{2n}^{(2)}$ Bethe equations (5.89) for small values of n and N and a generic value of η (namely, $\eta = -0.1i$) in Tables 5.1 - 5.6 for set I (5.13), and in Tables 5.7 - 5.12 for set II (5.14). [4] Each table also displays the cardinalities $(m_1, \ldots, m_n)$ of the Bethe roots, the corresponding

[4] The invariance of the Bethe equations under $u_k^{(l)} \mapsto u_k^{(l)} + 2\pi i$ and $u_k^{(l)} \mapsto -u_k^{(l)}$ can be used to restrict the Bethe roots to the domain $\Im m(u_k^{(l)}) \in [0, 2\pi)$ and $\Re e(u_k^{(l)}) \ge 0$.

Dynkin label $(a_1, \ldots, a_n)$ obtained using the formula (5.106), the degeneracy ("deg") of the corresponding eigenvalue of the Hamiltonians $\mathcal{H}^{(I)}$ and $\mathcal{H}^{(II)}$ (or, equivalently, of the transfer matrix $t(u)$ at some generic value of u) obtained by direct diagonalization, and the multiplicity ("mult") i.e., the number of solutions of the Bethe equations with the given cardinality of Bethe roots.

We observe that, for each solution of the Bethe equations in these tables, the dimension of the representation corresponding to the Dynkin label coincides with the degeneracy. [5] Moreover, the degeneracies and multiplicities predicted by the quantum group symmetry (5.65)-(5.67) and (5.85)-(5.87) are completely accounted for by the Bethe ansatz solutions. [6]

The eigenvalues of the Hamiltonians $\mathcal{H}^{(I)}$ (5.42) and $\mathcal{H}^{(II)}$ (5.52), as well as the eigenvalues of the transfer matrix $t(u)$ (5.18) for the two sets (5.13)-(5.14) at some generic value of u, are not displayed in the tables in order to minimize their size. Nevertheless, we have computed these eigenvalues both directly and from the reported solutions of the Bethe equations using (5.101) and (5.94)-(5.100), respectively; and we find perfect agreement between the results from these two approaches.

5.7 Conclusions

We have argued that the $A^{(2)}_{2n}$ integrable open quantum spin chains with the boundary conditions specified by (5.13) and (5.14) have the quantum group symmetries

[5] The dimensions corresponding to the Dynkin labels can be read off from (5.65)-(5.67) and (5.85)-(5.87), or more generally can be obtained from e.g. [98].

[6] The astute reader will notice that two solutions are missing from Table 5.12. We expect that this incompleteness can be attributed to our limited skill in finding solutions of nonlinear systems of 9 equations with 9 unknowns, and not to the non-existence of such solutions.

$U_q(B_n)$ and $U_q(C_n)$, respectively, see Eqs. (5.63) and (5.83). A key point of this argument is that the Hamiltonians can be expressed as sums of two-body terms, see (5.42) and (5.52). We have found a formula (5.106) for the Dynkin label of a Bethe state; the Dynkin label uniquely characterizes an irreducible representation, and in particular determines its dimension, which is the degeneracy of the corresponding eigenvalue. With the help of this formula, we have verified numerically (for a generic value of η) that the degeneracies and multiplicities implied by the quantum group symmetry (5.65)-(5.67) and (5.85)-(5.87) are completely accounted for by the Bethe ansatz solutions, see Tables 5.1 - 5.6 and 5.7 - 5.12, respectively. Similar results have recently been noted for the simpler case of the $U_q(A_1)$-invariant spin-1/2 chain [91] at generic values of q in [119].

Several interesting problems remain to be addressed, including the following: understanding further the realization of $U_q(C_n)$ specified by the nonstandard coproduct (5.77); proving that the transfer matrix $t(u)$ for the set II (5.14) has $U_q(C_n)$ symmetry; showing that the Bethe states have the highest weight property (5.105); and investigating the case that q is a root of unity (non-generic values of η). We also note that the sets (5.13) and (5.14) do not exhaust the possible integrable diagonal boundary conditions [93, 94]. We expect that models with these other boundary conditions will have "less" quantum group symmetry, which nevertheless may be worth exploring. It may also be interesting to find explicit formulas for the multiplicities in the tensor product decompositions of B_n (5.64) and C_n (5.84) in terms of the Dynkin labels $a_1, \ldots, a_n$.[7] These multiplicities should – remarkably – coincide with the number of

[7] For the case of A_1, such a formula is well known, see e.g. Eq. (2.8) in [119]. Some recent progress on this problem was reported in [120, 121].

solutions of the Bethe equations (5.89) at generic values of η for the corresponding (5.106) values of $m_1, \ldots, m_n$.

5.8 Appendix A: The $A_{2n}^{(2)}$ R-matrix

The R-matrix associated with the fundamental representation of $A_{2n}^{(2)}$ was found by Bazhanov [81, 82] and Jimbo [83]. We follow the latter reference; however, as in [99], we use the variables u and η instead of x and k, respectively, which are related as follows:

$$x = e^u \,, \qquad\qquad k = e^{2\eta} \,. \tag{5.114}$$

The R-matrix is given by [8]

$$\begin{aligned} R(u) &= c(u) \sum_{\alpha \ne \alpha'} e_{\alpha\alpha} \otimes e_{\alpha\alpha} + b(u) \sum_{\alpha \ne \beta, \beta'} e_{\alpha\alpha} \otimes e_{\beta\beta} \\ &+ \Big(e(u) \sum_{\alpha < \beta, \alpha \ne \beta'} + \bar{e}(u) \sum_{\alpha > \beta, \alpha \ne \beta'} \Big)\, e_{\alpha\beta} \otimes e_{\beta\alpha} + \sum_{\alpha\,, \beta} a_{\alpha\beta}(u)\, e_{\alpha\beta} \otimes e_{\alpha'\beta'} \,, \end{aligned} \tag{5.115}$$

with

$$\begin{aligned} c(u) &= 2\sinh(\frac{u}{2} - 2\eta)\ \cosh(\frac{u}{2} - (2n+1)\eta) \,, \\ b(u) &= 2\sinh(\frac{u}{2})\ \cosh(\frac{u}{2} - (2n+1)\eta) \,, \\ e(u) &= -2e^{-\frac{u}{2}}\sinh(2\eta)\ \cosh(\frac{u}{2} - (2n+1)\eta) \,, \\ \bar{e}(u) &= e^u e(u) \,, \end{aligned} \tag{5.116}$$

[8] This expression for the R-matrix differs from the one given in Ref. [83] by the overall factor $2e^{u+(2n+3)\eta}$.

$$a_{\alpha\beta}(u) = \begin{cases} \sinh(u-(2n-1)\eta)+\sinh((2n-1)\eta) & \alpha=\beta, \alpha\neq\alpha' \,, \\ \\ \sinh(u-(2n+1)\eta)+\sinh((2n+1)\eta)+ & \\ +\sinh((2n-1)\eta)-\sinh((2n+3)\eta) & \alpha=\beta, \alpha=\alpha' \,, \\ \\ -2e^{((2n+1)+2(\bar\alpha-\bar\beta))\eta}e^{-\frac{u}{2}}\sinh\frac{u}{2}\sinh(2\eta) & \alpha<\beta, \alpha\neq\beta' \,, \\ \\ 2e^{(2(2n+1)-2\beta+2)\eta}e^{-u}\sinh((2n+3-2\beta)\eta)\sinh(2\eta)- & \\ -2e^{((2n+3)-2\beta)\eta}\cosh((2(2n+2)-2\beta)\eta)\sinh(2\eta) & \alpha<\beta, \alpha=\beta' \,, \\ \\ 2e^{(-(2n+1)+2(\bar\alpha-\bar\beta))\eta}e^{\frac{u}{2}}\sinh\frac{u}{2}\sinh(2\eta) & \alpha>\beta, \alpha\neq\beta' \,, \\ \\ 2e^{u-2\beta\eta}\sinh(((2n+1)-2\beta)\eta)\sinh(2\eta)- & \\ -2e^{((2n+1)-2\beta)\eta}\cosh(2\beta\eta)\sinh(2\eta) & \alpha>\beta, \alpha=\beta' \,, \end{cases}$$

where

$$\bar\alpha = \begin{cases} \alpha+\frac{1}{2} & 1\leq\alpha<n+1 \\ \alpha & \alpha=n+1 \\ \alpha-\frac{1}{2} & n+1<\alpha\leq 2n+1 \end{cases} \,, \tag{5.117}$$

$$\alpha' = 2n+2-\alpha \,,$$

$$\alpha,\beta = 1\,,2\,,\ldots\,,2n+1\,. \tag{5.118}$$

This R-matrix has crossing symmetry (5.7), where V is given by [9]

$$V = \sum_{\alpha} e_{\alpha\alpha}\delta_{\alpha,\alpha'} + \sum_{\alpha<\alpha'} e^{[-(2n+1)+2\alpha]\eta}e_{\alpha\alpha'} + \sum_{\alpha>\alpha'} e^{(2n+1-2\alpha')\eta}e_{\alpha\alpha'}\,. \tag{5.119}$$

[9]We take this opportunity to correct several typos in the corresponding equation (59) in [99].

The matrix $M = V^t V$ is therefore given by the diagonal matrix

$$M = \mathrm{diag}(e^{4(n+1-\bar{\alpha})\eta})\,, \qquad \alpha = 1, 2, \ldots, 2n+1\,. \tag{5.120}$$

5.9 Appendix B: Eigenvalues of the Cartan generators

We sketch here a proof of the relation (5.108)

$$\begin{aligned} h_1 &= N - m_1\,, \\ h_i &= m_{i-1} - m_i\,, \qquad i = 2, 3, \ldots, n\,, \end{aligned} \tag{5.121}$$

based on the nested algebraic Bethe ansatz solution [100]. Since the argument is somewhat intricate, it is helpful to first consider some special cases. Hence, as a first warm-up, we consider the case $A_2^{(2)}$ in Section 5.9.1; and then, as a second warm-up, we consider the case $A_4^{(2)}$ in Section 5.9.2. Finally, we consider the general case $A_{2n}^{(2)}$ in Section 5.9.3. [10]

5.9.1 $A_2^{(2)}$

For the case $n = 1$, the Bethe states are given by

$$|\Lambda^{(m_1)}\rangle = B_2(u_1^{(1)}) \cdots B_2(u_{m_1}^{(1)})|0\rangle + \ldots\,, \tag{5.122}$$

where $B_2(u)$ is the operator appearing in the double-row monodromy matrix (5.103), and $|0\rangle$ is the reference state (5.104). The ellipsis denotes contributions from terms

[10] The proof of (5.121) presented here supersedes the discussion given in Appendix B of [99].

that also depend on the operator $F(u)$, which here and below we assume can be safely ignored. Using the facts [11]

$$[H_1\,, B_2(u)] = -B_2(u)\,, \qquad H_1|0\rangle = N|0\rangle\,, \tag{5.123}$$

we immediately see that

$$H_1|\Lambda^{(m_1)}\rangle = (N-m_1)|\Lambda^{(m_1)}\rangle\,. \tag{5.124}$$

Therefore $h_1 = N - m_1$, in agreement with (5.121).

5.9.2 $A_4^{(2)}$

We now consider the case $n = 2$, where nesting first appears. The (first-level) Bethe states are given by

$$|\Lambda^{(m_1,m_2)}\rangle = f_{i_1\cdots i_{m_1}} B_{i_1}(u_1^{(1)}) \cdots B_{i_{m_1}}(u_{m_1}^{(1)})|0\rangle + \ldots\,, \tag{5.125}$$

where $i_1, \ldots, i_{m_1} \in \{2,3,4\}$, $f_{i_1\cdots i_{m_1}}$ are coefficients that are still to be determined, and summation over repeated indices is understood.

Let n_i denote the number of $B_i(u)$ operators appearing in $|\Lambda^{(m_1,m_2)}\rangle$ (5.125). Evidently,

$$m_1 = n_2 + n_3 + n_4\,. \tag{5.126}$$

Using the facts

$$[H_1\,, B_j(u)] = -B_j(u)\,, \qquad j = 2,3,4\,, \qquad H_1|0\rangle = N|0\rangle\,, \tag{5.127}$$

[11] In order to lighten the notation, here and below we drop the notation $\Delta_{(k)}$ for the Cartan generators on k sites.

we obtain

$$H_1|\Lambda^{(m_1,m_2)}\rangle = (N - n_2 - n_3 - n_4)|\Lambda^{(m_1,m_2)}\rangle\,, \tag{5.128}$$

which, in view of (5.126), again implies $h_1 = N - m_1$.

Moreover, using the facts

$$[H_2\,, B_j(u)] = \begin{cases} B_j(u) & \text{for } j = 2 \\ -B_j(u) & \text{for } j = 4 \\ 0 & \text{otherwise} \end{cases}\,, \qquad H_2|0\rangle = 0\,, \tag{5.129}$$

we obtain

$$H_2|\Lambda^{(m_1,m_2)}\rangle = (n_2 - n_4)|\Lambda^{(m_1,m_2)}\rangle\,, \tag{5.130}$$

which implies

$$h_2 = n_2 - n_4\,. \tag{5.131}$$

The coefficients in (5.125) are given by the scalar product [12]

$$f_{i_1\cdots i_{m_1}} = \left(\langle e_{i_1}| \otimes \cdots \otimes \langle e_{i_{m_1}}|\right) |\tilde{\psi}\rangle\,, \tag{5.132}$$

where $|\tilde{\psi}\rangle$ is the second-level state

$$|\tilde{\psi}\rangle = \tilde{B}_2(u_1^{(2)}) \cdots \tilde{B}_2(u_{m_2}^{(2)})|\tilde{0}\rangle + \ldots \tag{5.133}$$

where $\tilde{B}_2(u)$ are the $A_2^{(2)}$ creation operators constructed as in (5.102) with $n = 1$ except with *inhomogeneous* monodromy matrices (the inhomogeneities are given by

[12]Since the transfer matrix is symmetric (see Appendix B in [102]), its left and right eigenvectors are each other's transpose.

$\{u_1^{(1)}, \ldots, u_{m_1}^{(1)}\}$). Moreover,

$$|\tilde{0}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^{\otimes m_1} , \tag{5.134}$$

and

$$|e_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \qquad |e_3\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} , \qquad |e_4\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} . \tag{5.135}$$

Let $\tilde{H}_1$ denote the Cartan generator for the case $A_2^{(2)}$, and let us now evaluate its matrix element

$$\left(\langle e_{i_1}| \otimes \cdots \otimes \langle e_{i_{m_1}}|\right) \tilde{H}_1 |\tilde{\psi}\rangle \tag{5.136}$$

in two different ways. To compute the action of $\tilde{H}_1$ to the right, we use $\tilde{H}_1|\tilde{\psi}\rangle = (m_1 - m_2)|\tilde{\psi}\rangle$, similarly to (5.124). To compute the action of $\tilde{H}_1$ to the left, we use the fact

$$\tilde{H}_1 |e_j\rangle = \begin{cases} |e_j\rangle & \text{for } j = 2 \\ -|e_j\rangle & \text{for } j = 4 \\ 0 & \text{otherwise} \end{cases} , \tag{5.137}$$

and therefore

$$\left(\langle e_{i_1}| \otimes \cdots \otimes \langle e_{i_{m_1}}|\right) \tilde{H}_1 = \left(\langle e_{i_1}| \otimes \cdots \otimes \langle e_{i_{m_1}}|\right) (n_2 - n_4) . \tag{5.138}$$

We conclude that

$$(n_2 - n_4)\, f_{i_1 \cdots i_{m_1}} = (m_1 - m_2)\, f_{i_1 \cdots i_{m_1}} , \tag{5.139}$$

which implies that $f_{i_1\cdots i_{m_1}}$ is zero unless

$$n_2 - n_4 = m_1 - m_2 \,. \tag{5.140}$$

Recalling (5.131), we conclude that $h_2 = m_1 - m_2$, in agreement with (5.121).

5.9.3 $A_{2n}^{(2)}$

In order to treat the general case, it is necessary to adopt a more systematic (but unfortunately significantly heavier) notation. We therefore write the Bethe states as

$$|\Lambda^{(m_1,\ldots,m_n)}\rangle = f^{(1)}_{i_1^{(1)}\cdots i_{m_1}^{(1)}} |\psi^{(1)}\rangle_{i_1^{(1)}\cdots i_{m_1}^{(1)}} \,. \tag{5.141}$$

5.9.3.1 First level

The first-level states are given by

$$|\psi^{(1)}\rangle_{i_1^{(1)}\cdots i_{m_1}^{(1)}} = B^{(1)}_{i_1^{(1)}}(u_1^{(1)}) \cdots B^{(1)}_{i_{m_1}^{(1)}}(u_{m_1}^{(1)})|0^{(1)}\rangle + \ldots \,, \tag{5.142}$$

where $i_1^{(1)}, \ldots, i_{m_1}^{(1)} \in \{2, \ldots, 2n\}$; and $B_i^{(1)}(u) \equiv B_i(u)$ and $|0^{(1)}\rangle \equiv |0\rangle$ are given by (5.103) and (5.104), respectively.

Letting $n_i^{(1)}$ denote the number of $B_i^{(1)}(u)$ operators appearing in (5.142), we have

$$m_1 = n_2^{(1)} + \ldots + n_{2n}^{(1)} \,. \tag{5.143}$$

For $H_i^{(1)} \equiv H_i$, we have for $i = 1$:

$$\left[H_1^{(1)}\,, B_j^{(1)}(u)\right] = -B_j^{(1)}(u)\,, \qquad j = 2, \ldots, 2n\,, \qquad H_1^{(1)}|0^{(1)}\rangle = N|0^{(1)}\rangle\,; \tag{5.144}$$

and for $i > 1$:

$$\left[H_i^{(1)}\,, B_j^{(1)}(u)\right] = \begin{cases} B_j^{(1)}(u) & \text{for } j = i \\ -B_j^{(1)}(u) & \text{for } j = 2n+2-i \\ 0 & \text{otherwise} \end{cases} \,, \qquad H_i^{(1)}|0^{(1)}\rangle = 0\,. \tag{5.145}$$

Therefore

$$\begin{aligned} H_1^{(1)}|\Lambda^{(m_1,\ldots,m_n)}\rangle &= (N - n_2^{(1)} - \ldots - n_{2n}^{(1)})\,|\Lambda^{(m_1,\ldots,m_n)}\rangle\,, \\ H_i^{(1)}|\Lambda^{(m_1,\ldots,m_n)}\rangle &= (n_i^{(1)} - n_{2n+2-i}^{(1)})\,|\Lambda^{(m_1,\ldots,m_n)}\rangle\,, \qquad i = 2,\ldots,n\,, \end{aligned} \tag{5.146}$$

which implies

$$\begin{aligned} h_1 &= N - m_1\,, \\ h_i &= n_i^{(1)} - n_{2n+2-i}^{(1)}\,, \qquad i = 2,\ldots,n\,. \end{aligned} \tag{5.147}$$

5.9.3.2 Second level

The coefficients in (5.141) are given by the scalar product

$$f^{(1)}_{i_1^{(1)}\cdots i_{m_1}^{(1)}} = \left(\langle e^{(1)}_{i_1^{(1)}}| \otimes \cdots \otimes \langle e^{(1)}_{i_{m_1}^{(1)}}|\right) |\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}}\, f^{(2)}_{i_1^{(2)}\cdots i_{m_2}^{(2)}}\,, \tag{5.148}$$

where the second-level states are given by

$$|\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}} = B^{(2)}_{i_1^{(2)}}(u_1^{(2)}) \cdots B^{(2)}_{i_{m_2}^{(2)}}(u_{m_2}^{(2)})|0^{(2)}\rangle + \ldots\,, \tag{5.149}$$

where $i_1^{(2)}, \ldots, i_{m_2}^{(2)} \in \{2, \ldots, 2n-2\}$; $B_i^{(2)}(u)$ are the (inhomogeneous) creation operators for $A_{2n-2}^{(2)}$; and

$$|0^{(2)}\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{2n-1}^{\otimes m_1}\,. \tag{5.150}$$

Moreover,

$$|e_2^{(1)}\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{2n-1} , \qquad \ldots \qquad , \qquad |e_{2n}^{(1)}\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}_{2n-1} . \tag{5.151}$$

We have that

$$m_2 = n_2^{(2)} + \ldots + n_{2n-2}^{(2)} , \tag{5.152}$$

and hence

$$\begin{aligned} H_1^{(2)}|\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}} &= (m_1 - m_2)\,|\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}} , \\ H_i^{(2)}|\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}} &= (n_i^{(2)} - n_{2n-i}^{(2)})\,|\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}} , \qquad i = 2, \ldots, n-1 . \end{aligned} \tag{5.153}$$

Furthermore,

$$H_i^{(2)}|e_j^{(1)}\rangle = \begin{cases} |e_j^{(1)}\rangle & \text{for } j = i+1 \\ -|e_j^{(1)}\rangle & \text{for } j = 2n+1-i \\ 0 & \text{otherwise} \end{cases} . \tag{5.154}$$

Evaluating the matrix element

$$\left(\langle e_{i_1^{(1)}}^{(1)}| \otimes \cdots \otimes \langle e_{i_{m_1}^{(1)}}^{(1)}| \right) H_i^{(2)}|\psi^{(2)}\rangle_{i_1^{(2)}\cdots i_{m_2}^{(2)}}\, f^{(2)}_{i_1^{(2)}\cdots i_{m_2}^{(2)}} \tag{5.155}$$

in two different ways by acting with $H_i^{(2)}$ to both the left and the right, we obtain for $i = 1$

$$n_2^{(1)} - n_{2n}^{(1)} = m_1 - m_2 , \tag{5.156}$$

and for $i > 1$

$$n_{i+1}^{(1)} - n_{2n+1-i}^{(1)} = n_i^{(2)} - n_{2n-i}^{(2)} , \qquad i = 2, \ldots, n-1 . \tag{5.157}$$

5.9.3.3 Level k

At level $k = 2, 3, \ldots, n-1$, we have

$$f^{(k-1)}_{i_1^{(k-1)} \cdots i_{m_{k-1}}^{(k-1)}} = \left(\langle e^{(k-1)}_{i_1^{(k-1)}} | \otimes \cdots \otimes \langle e^{(k-1)}_{i_{m_{k-1}}^{(k-1)}} | \right) |\psi^{(k)}\rangle_{i_1^{(k)} \cdots i_{m_k}^{(k)}} \, f^{(k)}_{i_1^{(k)} \cdots i_{m_k}^{(k)}} \,, \tag{5.158}$$

where the level-k states are given by

$$|\psi^{(k)}\rangle_{i_1^{(k)} \cdots i_{m_k}^{(k)}} = B^{(k)}_{i_1^{(k)}}(u_1^{(k)}) \cdots B^{(k)}_{i_{m_k}^{(k)}}(u_{m_k}^{(k)}) |0^{(k)}\rangle + \ldots \,, \tag{5.159}$$

where $i_1^{(k)}, \ldots, i_{m_k}^{(k)} \in \{2, \ldots, 2n-2k+2\}$; $B_i^{(k)}(u)$ are the (inhomogeneous) creation operators for $A^{(2)}_{2n-2k+2}$; and

$$|0^{(k)}\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{2n-2k+3}^{\otimes m_{k-1}} \,. \tag{5.160}$$

Moreover,

$$|e_2^{(k-1)}\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}_{2n-2k+3} \,, \quad \ldots \quad , \quad |e^{(k-1)}_{2n-2k+4}\rangle = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}_{2n-2k+3} \,. \tag{5.161}$$

We have that

$$m_k = n_2^{(k)} + \ldots + n^{(k)}_{2n-2k+2} \,. \tag{5.162}$$

Also,

$$\left[H_1^{(k)} \,, B_j^{(k)}(u) \right] = -B_j^{(k)}(u) \,, \quad j = 2, \ldots, 2n-2k+2 \,, \quad H_1^{(k)} |0^{(k)}\rangle = m_{k-1} |0^{(k)}\rangle \,; \tag{5.163}$$

and for $i > 1$:

$$\left[H_i^{(k)}\,,B_j^{(k)}(u)\right] = \begin{cases} B_j^{(k)}(u) & \text{for } j = i \\ -B_j^{(k)}(u) & \text{for } j = 2n-2k+4-i \\ 0 & \text{otherwise} \end{cases} \quad , \; H_i^{(k)}|0^{(k)}\rangle = 0\,. \tag{5.164}$$

Hence

$$\begin{aligned} H_1^{(k)}|\psi^{(k)}\rangle_{i_1^{(k)}\ldots i_{m_k}^{(k)}} &= (m_{k-1}-m_k)\,|\psi^{(k)}\rangle_{i_1^{(k)}\ldots i_{m_k}^{(k)}}\,, \qquad (5.165)\\ H_i^{(k)}|\psi^{(k)}\rangle_{i_1^{(k)}\ldots i_{m_k}^{(k)}} &= (n_i^{(k)} - n_{2n-2k+4-i}^{(k)})\,|\psi^{(k)}\rangle_{i_1^{(k)}\ldots i_{m_k}^{(k)}}\,, \qquad i = 2,\ldots,n-k+1\,. \end{aligned}$$

Furthermore,

$$H_i^{(k)}|e_j^{(k-1)}\rangle = \begin{cases} |e_j^{(k-1)}\rangle & \text{for } j = i+1 \\ -|e_j^{(k-1)}\rangle & \text{for } j = 2n-2k+5-i \\ 0 & \text{otherwise} \end{cases} \;. \tag{5.166}$$

Evaluating the matrix element

$$\left(\langle e_{i_1^{(k-1)}}^{(k-1)}| \otimes \cdots \otimes \langle e_{i_{m_{k-1}}^{(k-1)}}^{(k-1)}|\right) H_i^{(k)}|\psi^{(k)}\rangle_{i_1^{(k)}\ldots i_{m_k}^{(k)}}\, f_{i_1^{(k)}\ldots i_{m_k}^{(k)}}^{(k)} \tag{5.167}$$

in two different ways by acting with $H_i^{(k)}$ to both the left and the right, we obtain

$$\begin{aligned} n_2^{(k-1)} - n_{2n-2k+4}^{(k-1)} &= m_{k-1} - m_k\,, \\ n_{i+1}^{(k-1)} - n_{2n-2k+5-i}^{(k-1)} &= n_i^{(k)} - n_{2n-2k+4-i}^{(k)}\,, \qquad i = 2,\ldots,n-k+1\,. \end{aligned} \tag{5.168}$$

5.9.3.4 Level n

At the final level $k = n$, we have

$$f_{i_1^{(n-1)}\ldots i_{m_{n-1}}^{(n-1)}}^{(n-1)} = \left(\langle e_{i_1^{(n-1)}}^{(n-1)}| \otimes \cdots \otimes \langle e_{i_{m_{n-1}}^{(n-1)}}^{(n-1)}|\right) |\psi^{(n)}\rangle\,, \tag{5.169}$$

where the level-n states are given by

$$|\psi^{(n)}\rangle = B_2^{(n)}(u_1^{(n)}) \cdots B_2^{(n)}(u_{m_n}^{(n)})|0^{(n)}\rangle + \ldots\,, \tag{5.170}$$

where $B_i^{(n)}(u)$ are the (inhomogeneous) creation operators for $A_2^{(2)}$. Moreover,

$$|0^{(n)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}^{\otimes m_{n-1}}\,, \tag{5.171}$$

and

$$|e_2^{(n-1)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\,, \qquad |e_3^{(n)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\,, \qquad |e_4^{(n)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}\,. \tag{5.172}$$

We have that

$$H_1^{(n)}|\psi^{(n)}\rangle = (m_{n-1} - m_n)\,|\psi^{(n)}\rangle \tag{5.173}$$

and

$$H_1^{(n)}|e_j^{(n-1)}\rangle = \begin{cases} |e_j^{(n-1)}\rangle & \text{for } j = 2 \\ -|e_j^{(n-1)}\rangle & \text{for } j = 4 \\ 0 & \text{otherwise} \end{cases}\,. \tag{5.174}$$

Evaluating the matrix element

$$\left(\langle e_{i_1^{(n-1)}}^{(n-1)}| \otimes \cdots \otimes \langle e_{i_{m_{n-1}}^{(n-1)}}^{(n-1)}|\right) H_1^{(n)}|\psi^{(n)}\rangle \tag{5.175}$$

in two different ways, we obtain

$$n_2^{(n-1)} - n_4^{(n-1)} = m_{n-1} - m_n\,. \tag{5.176}$$

Combining all the results (5.147), (5.156), (5.157), (5.168), (5.176), we obtain the desired relations (5.121). Indeed, one can see that

$$h_i = n^{(k-1)}_{i+2-k} - n^{(k-1)}_{2n+4-k-i}\,, \qquad k = 2, \ldots, n\,, \tag{5.177}$$

which gives for $i = k$

$$h_k = n^{(k-1)}_2 - n^{(k-1)}_{2n-2k+4} = m_{k-1} - m_k\,, \tag{5.178}$$

where the second equality follows from (5.168).

m_1	a_1	deg	mult	$\{u_k^{(1)}\}$
0	4	5	1	-
1	2	3	1	0.201347
2	0	1	1	$0.627218 \pm 1.28621i$

Table 5.1: B_1, $N = 2$

m_1	a_1	deg	mult	$\{u_k^{(1)}\}$
0	6	7	1	-
1	4	5	2	0.115986 0.351133
2	2	3	3	$0.524753 \pm 1.38161i$ $0.11483\,,\ 1.56044i$ $0.343261\,,\ 1.64011i$
3	0	1	1	$0.115223\,,\ 0.344343\,,\ 0.324313\ + i\pi$

Table 5.2: B_1, $N = 3$

m_1	m_2	a_1	a_2	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$
0	0	2	0	14	1	-	-
1	0	0	2	10	1	0.201347	-
2	2	0	0	1	1	$0.427307 \pm 0.971435i$	$0.506682 \pm 1.38565i$

Table 5.3: B_2, $N = 2$

m_1	m_2	a_1	a_2	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$
0	0	3	0	30	1	-	-
1	0	1	2	35	2	0.115986 0.351133	- -
2	1	0	2	10	1	$0.115986\,,\ 0.351133$	0.331791
2	2	1	0	5	3	$0.338012\,,\ 1.11733i$ $0.390693 \pm 1.11745i$ $0.113154\,,\ 1.01242i$	$0.340113 \pm 1.32976i$ $0.434061 \pm 1.4248i$ $0.410526 \pm 1.3294i$

Table 5.4: B_2, $N = 3$

m_1	m_2	m_3	a_1	a_2	a_3	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$	$\{u_k^{(3)}\}$
0	0	0	2	0	0	27	1	-	-	-
1	0	0	0	1	0	21	1	0.201347	-	-
2	2	2	0	0	0	1	1	$0.327207 \pm 0.786874i$	$0.372666 \pm 1.12783i$	$0.415697 \pm 1.42783i$

Table 5.5: B_3, $N = 2$

m_1	m_2	m_3	a_1	a_2	a_3	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$	$\{u_k^{(3)}\}$
0	0	0	3	0	0	77	1	-	-	-
1	0	0	1	1	0	105	2	0.115986 0.351133	- -	- -
2	1	0	0	0	2	35	1	0.115986 , 0.351133	0.331791	-
2	2	2	1	0	0	7	3	0.110446 , $0.776613i$ 0.335123 , $0.905482i$ $0.308473 \pm$ $0.927961i$	$0.287874 \pm$ $1.03712i$ $0.186397 \pm$ $1.03899i$ $0.333096 \pm$ $1.19533i$	$0.387205 \pm$ $1.40363i$ $0.327378 \pm$ $1.40468i$ $0.358468 \pm$ $1.44765i$

Table 5.6: B_3, $N = 3$

m_1	a_1	deg	mult	$\{u_k^{(1)}\}$
0	2	3	1	-
1	1	2	2	0.185137 1.04997
2	0	1	2	$0.757565 \pm 0.363991i$ $0.206122\,,\ 2.59788i$

Table 5.7: C_1, $N = 2$

m_1	a_1	deg	mult	$\{u_k^{(1)}\}$
0	3	4	1	-
1	2	3	3	0.111524 0.315352 1.38581
2	1	2	5	$1.10381 \pm 0.414939i$ 0.116934 , 0.776633 0.454616 , 0.531061 $0.117801\,,\ 2.59116i$ $0.369036\,,\ 2.73713i$
3	0	1	4	$0.886562\,,\ 0.777865 \pm 0.638435i$ $0.417895\,,\ 0.773051\,,\ 2.5569i$ $0.119916\,,\ 0.88464\,,\ 2.47305i$ $0.113539\,,\ 0.333831\,,\ 0.365549 + i\pi$

Table 5.8: C_1, $N = 3$

m_1	m_2	a_1	a_2	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$
0	0	2	0	10	1	-	-
1	0	0	1	5	1	0.201347	-
1	1	1	0	4	2	1.18368 0.18784	1.35557 0.716566
2	2	0	0	1	2	$0.844939 \pm 0.400816i$ $0.211755\,,\ 1.48557i$	$1.07213 \pm 0.422759i$ $0.714804i\,,\ 2.1946i$

Table 5.9: C_2, $N = 2$

m_1	m_2	a_1	a_2	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$
0	0	3	0	20	1	-	-
1	0	1	1	16	2	0.115986 0.351133	- -
1 , N=2	1	2	0	10	3	1.58467 0.321003 0.112316	1.70996 0.760756 0.701168
2	1	0	1	5	3	0.382283 , 0.963791 0.118089 , 1.05603 0.113785 , 0.333555	1.34441 1.3902 0.2923
2	2	1	0	4	6	0.397606 , 0.688759 $1.23957 \pm$ $0.466025i$ 0.119249 , $1.66217i$ 0.116831 , 0.865494 0.385256 , $1.71269i$ 0.117124 , 0.362471	$0.9169 \pm$ $0.307663i$ $1.39288 \pm$ $0.481069i$ $0.711593i$, $2.20269i$ $0.934114 \pm$ $0.250442i$ $0.61563i$, $2.28518i$ 0.34741 , $2.68405i$
3	3	0	0	1	4	0.989238 , $0.860023 \pm$ $0.700064i$ 0.425069 , 0.848958 , $1.5453i$ 0.113851 , 0.338372 , $1.44183i$ 0.120953 , 0.94247 , $1.51754i$	1.18442 , $1.06721 \pm$ $0.745089i$ 1.13679 , $0.680288i$, $2.20976i$ $0.279454 \pm$ $0.211351i$, $2.39497i$ 1.1893 , $0.757077i$, $2.14786i$

Table 5.10: C_2, $N = 3$

m_1	m_2	m_3	a_1	a_2	a_3	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$	$\{u_k^{(3)}\}$
0	0	0	2	0	0	21	1	-	-	-
1	0	0	0	1	0	14	1	0.201347	-	-
1	1	1	1	0	0	6	2	0.190268 1.35599	0.796966 1.55753	1.04547 1.68531
2	2	2	0	0	0	1	2	$0.9507 \pm$ $0.448287i$ $0.219256\,,$ $1.14053i$	$1.21099 \pm$ $0.473011i$ $0.543566i\,,$ $1.60164i$	$1.36739 \pm$ $0.485421i$ $0.885636i\,,$ $2.04527i$

Table 5.11: C_3, $N = 2$

m_1	m_2	m_3	a_1	a_2	a_3	deg	mult	$\{u_k^{(1)}\}$	$\{u_k^{(2)}\}$	$\{u_k^{(3)}\}$
0	0	0	3	0	0	56	1	-	-	-
1	0	0	1	1	0	64	2	0.115986 0.351133	- -	- -
1	1	1	2	0	0	21	3	0.113011 0.326182 1.86199	0.78232 0.839331 2.01428	1.03469 1.07712 2.10901
2	1	0	0	0	1	14	1	0.115986 , 0.351133	0.331791	-
2	1	1	0	1	0	14	3	0.117608 , 1.20956 0.11417 , 0.336229 0.372422 , 1.13284	1.58891 0.298556 1.54735	1.71382 0.751895 1.67608
2	2	2	1	0	0	6	6	0.377177 , 0.835326 $1.41135 \pm 0.538002i$ 0.409958 , $1.35937i$ 0.116641 , 0.980323 0.118386 , 0.376545 0.121155 , $1.30785i$	$1.03506 \pm 0.320648i$ $1.59277 \pm 0.555019i$ $0.414206i$, $1.74096i$ $1.05068 \pm 0.260276i$ 0.367 , $1.49213i$ $0.572787i$, $1.67608i$	$1.23102 \pm 0.37667i$ $1.70587 \pm 0.566549i$ $0.791369i$, $2.1359i$ $1.24798 \pm 0.342251i$ $0.65911i$, $2.2416i$ $0.885614i$, $2.04744i$
3	3	3	0	0	0	1	4	0.443222 , 0.937877 , $1.23794i$ 1.11346 , $0.953596 \pm 0.779036i$? ?	1.24501 , $0.44955i$, $1.66845i$ 1.3403 , $1.18988 \pm 0.830487i$? ?	1.41773 , $0.832685i$, $2.09128i$ 1.47811 , $1.32949 \pm 0.861223i$? ?

Table 5.12: C_3, $N = 3$

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