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

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Received 27 October 2013
Accepted for publication 6 December 2013
Published 20 December 2013

Abstract
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.

Keywords: integrable quantum spin chain, integrable boundary conditions, Bethe ansatz, boundary (surface) energy, Richardson–Gaudin model
PACS numbers: 75.10.Jm, 02.30.Ik, 03.65.Fd

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

1. Introduction

Ever since the open spin-1/2 XXX (isotropic) quantum spin chain with non-diagonal boundary terms was shown to be integrable [1–3], 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 [4] (see also [5]). A simplified version of this solution was subsequently shown to produce all the eigenvalues [6]. A beautiful expression for the corresponding eigenvectors was then proposed in [7]. Another simple solution was found and shown to be complete in [8].
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 ($\xi$) of the non-diagonal boundary term goes to zero, and compute the leading correction (of order $\xi^2$) 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 2 we briefly describe the model and recall its Bethe ansatz solution. In section 3 we present the computation of the boundary energy. Our conclusions are presented in section 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 [4], we take as our Hamiltonian

$$H = \sum_{n=1}^{N-1} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} + \frac{1}{q} (\sigma^z_n + \xi \sigma^x_n) + \frac{1}{p} \sigma^z_N,$$

where $p, q, \xi$ are arbitrary real boundary parameters. We consider the solution based on the following linear $T-Q$ equation [6]:

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

where $\Lambda(\lambda)$ is an eigenvalue of the model’s transfer matrix [1, 3, 4]. Moreover,

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

and

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

The zeros $\lambda_1, \ldots, \lambda_N$ of $Q(\lambda)$ satisfy the Bethe equations that follow directly from (2):

$$e_1(u_j)^{2N} e_2(p-1)(u_j)e_2(q-1)(u_j) - \prod_{k \neq j}^{N} e_2(u_j - u_k) e_2(u_j + u_k) = \pm \left(1 - \frac{1}{\sqrt{1 + \xi^2}}\right)^{2N},$$

$$\times \frac{u_j(u_j + \frac{i}{2})^{2N}}{(u_j - i(p - \frac{1}{2}))(u_j - i(q - \frac{1}{2})) \prod_{k=1}^{N} (u_j - u_k - i)(u_j + u_k - i)},$$

$$j = 1, 2, \ldots, N,$$

where

$$u_j = i (\lambda_j + \frac{1}{2}), \quad \bar{q} = \frac{q}{\sqrt{1 + \xi^2}}, \quad e_n(u) = \frac{u + \frac{i n}{2}}{u - \frac{i n}{2}}$$

$$n = 0, 1, 2, \ldots, N.$$
The eigenvalues of the Hamiltonian (1) are given by [6]

$$E = -2 \sum_{j=1}^{N} \frac{1}{u_j^2 + \frac{1}{4}} + N - 1 + \frac{1}{p} + \frac{1}{q}. $$  \hspace{1cm} (7)

We observe that the energy is invariant under $\xi \rightarrow -\xi$, 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 (1) can be changed by a global $\text{SU}(2)$ transformation (namely, rotation by $\pi$ about the $y$ axis, which leaves $\sigma^z$ invariant, but changes $\sigma^{x,z} \rightarrow -\sigma^{x,z}$). For definiteness, we shall further restrict to even values of $N$, and $p < 0$.

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

$$H_{\text{periodic}} = \sum_{n=1}^{N} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1}, \quad \vec{\sigma}_{N+1} = \vec{\sigma}_1, $$  \hspace{1cm} (8)

the ground-state energy $E_{0}^{\text{periodic}}(N)$ for large $N$ is given by

$$E_{0}^{\text{periodic}}(N) = N \epsilon_{\text{in}} + O \left( \frac{1}{N} \right), $$  \hspace{1cm} (9)

where $\epsilon_{\text{in}} = 1 - 4 \ln 2$. In contrast, for the open chain Hamiltonian (1), the ground-state energy $E_{0}(N; p, q, \xi)$ for large $N$ is given by (see, e.g. [9, 10])

$$E_{0}(N; p, q, \xi) = N \epsilon_{\text{in}} + E_{b}(p, q, \xi) + O \left( \frac{1}{N} \right), $$  \hspace{1cm} (10)

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

$$E_{b}(p, q, \xi) = \lim_{N \rightarrow \infty} \left[ E_{0}(N; p, q, \xi) - E_{0}^{\text{periodic}}(N) \right]. $$  \hspace{1cm} (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 (1) become diagonal, and the exact boundary energy is known [11–14],

$$E_{b}(p, q, \xi = 0) = \frac{1}{p} + \frac{1}{q} - 1 + \pi - 2 \int_{0}^{\infty} dx \frac{e^{-(2q-1)x} - e^{(2p-1)x} + e^{-x}}{\cosh x} $$

$$= \frac{1}{p} + \frac{1}{q} - 1 + \pi - \ln 4 + \psi \left( \frac{q}{2} \right) - \psi \left( \frac{1 + q}{2} \right) $$

$$+ \psi \left( \frac{2 - p}{2} \right) - \psi \left( \frac{1 - p}{2} \right), $$  \hspace{1cm} (12)

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

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

$$E_{b}(p, q, \xi) = E_{b}(p, q, \xi = 0) + E_{b}^{(1)}(p, q) \xi^2 + O(\xi^4), $$  \hspace{1cm} (13)

which contains only even powers of $\xi$ since the energy is invariant under $\xi \rightarrow -\xi$. 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 [6]), we find that the $N$ Bethe roots $\{u_1, \ldots, u_N\}$ describing the ground-state split evenly into two sets as $\xi \rightarrow 0$: ‘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 figure 1. We now proceed to consider separately the contributions to $E_{b}^{(1)}(p, q)$ from these two sets of roots.
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 reduction of the exact Bethe equations (5), namely,

$$e_1(v_j)^{2N}e_{2p-1}(v_j)e_{2q-1}(v_j) = \prod_{k \neq j}^{N/2} e_2(v_j - v_k) e_2(v_j + v_k), \quad j = 1, \ldots, \frac{N}{2}. \quad (14)$$

These roots still depend on $\xi$ 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 (14). We find that the agreement is very good for small values of $\xi$, as shown in figure 2.

The contribution of these small roots to the boundary energy is given by (12) with $q$ replaced by $\tilde{q}$. Expanding this result in powers of $\xi$, we recover the $\xi$-independent term $E_b(p, q, \xi = 0)$ in (13), and we obtain from the term of order $\xi^2$ the following contribution to $E_b^{(1)}(p, q)$ from the small roots:

$$E_b^{(1)}\text{small}(p, q) = \frac{1}{2q} - \frac{q}{4} \left[ \psi \left( \frac{q}{2} \right) - \psi \left( \frac{q + 1}{2} \right) \right]. \quad (15)$$

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 (5) to first order in $\xi$ using

$$\frac{a + b}{a - b} = 1 + \frac{2b}{a} + O\left( \left( \frac{b}{a} \right)^2 \right), \quad |a| \gg |b|. \quad (16)$$

We obtain

$$(p + q - 1) \frac{1}{w_j} = \sum_{k \neq j}^{N/2} \left( \frac{1}{w_j - w_k} + \frac{1}{w_j + w_k} \right) + \frac{1}{4} \xi^2 w_j \prod_{k \neq j}^{N/2} \frac{1}{1 - \left( \frac{w_k}{w_j} \right)^2}, \quad j = 1, \ldots, \frac{N}{2}. \quad (17)$$
These equations have some resemblance to those appearing in the Richardson–Gaudin models [15, 16]. However, the final term, which is due to the inhomogeneous term in the $T$-$Q$ equation (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. [9, 17–20].) To this end, we introduce the polynomial $q(w)$ of degree $N$ with zeros $\pm w_k$,

$$q(w) \equiv \prod_{k=1}^{N/2} (w - w_k)(w + w_k), \quad (18)$$

which has the asymptotic behavior

$$q(w) \sim w^N \quad \text{for} \quad w \to \infty. \quad (19)$$

We observe the identities

$$\frac{q''(w_j)}{q'(w_j)} = \frac{1}{w_j} + 2 \sum_{k \neq j} \left( \frac{1}{w_j - w_k} + \frac{1}{w_j + w_k} \right), \quad (20)$$

and

$$q'(w_j) = 2w_j^{N-1} \prod_{k \neq j} \left[ 1 - \left( \frac{w_k}{w_j} \right)^2 \right]. \quad (21)$$
where the prime denotes differentiation with respect to $w$. It follows that (17) is equivalent to
\begin{equation}
 w_j q''(w_j) - (2p + 2q - 1) q'(w_j) + \xi^2 w_j^{N+1} = 0.
\end{equation}
(22)
The equation obtained by replacing $w_j$ with $-w_j$ in (22) is consistent with (22), since $q''(-w_j) = q''(w_j)$, $q'(-w_j) = -q'(w_j)$, and $N$ is even. Therefore, the function
\[ w q''(w) - (2p + 2q - 1) q'(w) + \xi^2 w^{N+1} \]
has all the zeros of $q(w)$, and is a polynomial of degree $N + 1$. It follows that
\begin{equation}
 w q''(w) - (2p + 2q - 1) q'(w) + \xi^2 w^{N+1} - \xi^2 w q(w) = 0.
\end{equation}
(24)
Remarkably, the unusual term in the Richardson–Gaudin-type equations (17) (that originated from the inhomogeneous term in the $T$-$Q$ equation (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
\[ x_j = w_j \xi, \quad x = w \xi, \]
and the corresponding polynomial
\begin{equation}
 g(x) = \prod_{k=1}^{\xi} (x - x_k)(x + x_k).
\end{equation}
(25)
Evidently, $q(w) = \xi^{-N} g(x)$, and therefore (24) becomes
\begin{equation}
 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.
\end{equation}
(27)
Note that the $\xi$ dependence has disappeared. This equation (or, equivalently, equation (24)) can be easily solved numerically for the zeros of $g(x)$ even for large values of $N$, as shown in the example of figure 3.

We observe that the term $\frac{x^{N+1}}{g(x)}$ in (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 (27) can be written as

\[
 x \left( \frac{dG(x)}{dx} + G(x)^2 - 1 \right) - (2p + 2q - 1)G(x) = 0, \quad (x \approx 0),
\]

where

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

The contribution of the large roots to the energy (7) can be expressed in terms of the derivative of \( G(x) \) at \( x = 0 \):

\[
 E_{\text{large}} = \frac{1}{2} \sum_{j=1}^{N} \left[ \psi \left( \frac{q+1}{2} \right) - \psi \left( \frac{q}{2} \right) \right] + \frac{1}{2} \frac{dG(x)}{dx} \bigg|_{x=0}.
\]

The first-order differential equation (28) can be solved in closed form

\[
 G(x) = \frac{1}{x} \left[ J_{p+q-1}(-ix) + CY_{p+q-1}(-ix) \right] - \frac{1}{x} \left[ J_{p+q}(-ix) + CY_{p+q}(-ix) \right],
\]

where \( J_p(x) \) and \( Y_p(x) \) 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 \( p + q \leq 0 \) and \( p + q \neq -1/2 \), then \( C = 0 \).

One way to evaluate (31) is to expand the Bessel functions in (32) about \( x = 0 \) and obtain the \( O(x) \) term. Even easier is to substitute \( G(x) = ax + O(x^2) \) into (28) and solve for the constant \( a \). We obtain

\[
 E_{b}^{(1) \text{large}}(p, q) = \frac{1}{2(1 - p - q)}. \tag{33}
\]

In deriving the result (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 \( \xi \) is small), as shown for \( N = 8 \) in figure 4.

### 3.3. Final result

Adding the results from the small roots (15) and the large roots (33), we obtain our final result for the leading correction to the boundary energy (defined in equation (13))

\[
 E_{b}^{(1)}(p, q) = E_{b}^{(1) \text{small}}(p, q) + E_{b}^{(1) \text{large}}(p, q)
 = \frac{1}{2q} - \frac{q}{4} \left[ \psi \left( \frac{q}{2} \right) - \psi \left( \frac{q+1}{2} \right) \right] + \frac{1}{2(1 - p - q)}. \tag{34}
\]

We have already noted in figures 2 and 4 some partial checks using numerical results for \( N = 8 \). In principle, the final result (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 [10] using extrapolation with values of \( N \) up to 256. However, we have not (yet) managed to accurately solve the exact Bethe equations (5) numerically for the ground-state Bethe roots with such large values of \( N \).
Figure 4. The energy from the exact large roots \( E^{(1)\text{large}}(N) \) for \( N = 8 \) is plotted with red circles; the \( N \to \infty \) result \( E^{(1)\text{large}}_p(p, q) \xi^2 \), with \( E_{p, q}^{(1)\text{large}} \) given by (33), is the blue curve. In (a), \( p = -8, q = 4 \) and \( \xi \) is varied; in (b), \( p = -8, \xi = 1/8 \) and \( q \) is varied; in (c), \( q = 4, \xi = 1/8 \) and \( p \) is varied.

4. Conclusion

We have argued that the recently-found Bethe ansatz solution [4, 6] of the model (1) can be used to perform a computation in the thermodynamic limit. Indeed, at least for small values of \( \xi \), the inhomogeneous term in the T-Q equation (2), which leads to an unusual term in the Richardson–Gaudin-type equations (17) for the large roots, does not impede the derivation of an analytical expression (34) for the boundary energy. It would be interesting if one could pass directly from the T-Q equation (2) to the T-Q-type equation (24), without first going through the equations (17).

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

Acknowledgments

This work was supported in part by the National Science Foundation under Grant PHY-1212337, and by a Cooper fellowship.

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