Published by Institute of Physics Publishing for SISSA

Received: *April 19, 2007*
Accepted: *May 15, 2007*
Published: *May 21, 2007*

Finite-size correction and bulk hole-excitations for special case of an open XXZ chain with nondiagonal boundary terms at roots of unity

Rajan Murgan

Physics Department, P.O. Box 248046, University of Miami,
Coral Gables, FL 33124, U.S.A.
E-mail: rmurgan@physics.miami.edu

Abstract: Using our solution for the open spin-1/2 XXZ quantum spin chain with N spins and two arbitrary boundary parameters at roots of unity, the central charge and the conformal dimensions for bulk hole excitations are derived from the $1/N$ correction to the energy (Casimir energy).

Keywords: Lattice Integrable Models, Bethe Ansatz, Boundary Quantum Field Theory.

Contents

1. Introduction

The integrable open spin-1/2 XXZ chain has been subjected to intensive studies due to its growing applications in various fields of physics, e.g., statistical mechanics, string theory and condensed matter physics. However, obtaining exact solutions for this model has been a rather challenging and elusive task for many years. Various progress have been made in obtaining solutions for this model, either using the Bethe ansatz approach for diagonal [1]–[4], constrained nondiagonal [5]–[9] and nondiagonal cases at roots of unity [10]–[13], or using the representation theory of the q-Onsager algebra for general nondiagonal cases [14]. Approaches based on boundary Temperley-Lieb algebra and its representations have also been presented recently, from which the spectral properties of the chain have been studied [15]. Upon obtaining the desired solution, the next natural question that needed to be addresed is its practicality within various contexts. One important area where these solutions have found creditable applications is in determining finite size corrections to the ground state energy. By relating to conformal invariance, these finite size corrections are shown to be related directly to other crucial parameters like the critical indices, central charge and conformal dimensions [17]–[20]. There are few methods and approaches to accomplish this task. De Vega and Woynarowich [21] derived integral equations for calculating leading finite-size corrections for models solvable by Bethe Ansatz approach [22]. This was then generalized to nested Bethe Ansatz models as well [23]. Another approach was introduced by Woynarowich and Eckel [24, 25], which utilizes Euler-Maclaurin formula and Wiener-Hopf integration to compute these corrections for the closed XXZ chain. Others have also studied more general integrable spin chain models e.g., XXZ diagonal [2, 3],

JHEP05(2007)069

nondiagonal cases [28], quantum spin 1/2 chains with non-nearest-neighbour short-range interaction [26] and XXZ$(1/2, 1)$ which contains alternating spins of 1/2 and 1 [27], within similar framework. Other approaches e.g., based on NLIE (Nonlinear Integral Equations) have also been successful in determining these effects for integrable lattice models [29] and related integrable quantum field theories, such as the sine-Gordon model with periodic [30]–[32], Dirichlet [33]–[37] and Neumann boundary conditions [28, 42].

With similar aim in mind, utilizing an exact solution for the integrable spin-1/2 XXZ chain with nondiagonal boundary terms at roots of unity we found earlier for even number of sites [11, 38],[1] and extending the solution to account for odd number of sites as well, we compute the correction of order $1/N$ (Casimir energy) to the ground state energy together with its low lying excited states (multi-hole states). We employ the method introduced by Woynarovich and Eckle [24] that makes use of Euler-Maclaurin formula [45] and Wiener-Hopf integration [46]. In particular, we compute the analytical expressions for central charge and the conformal dimensions of low lying excited states. We also compare these analytical results to corresponding numerical results obtained by solving the model numerically for some large number of sites.

The outline of this article is as follows. In section 2, we review the Bethe Ansatz solution [11, 38]. We also present an extension of that result to include solution for odd N. In section 3, we present the calculation of $1/N$ correction to the ground state energy and hence our results for the central charge and conformal dimensions of low lying excited states. We notice that the lowest energy state for even N of this model has one hole. Hence, the true ground state (lowest energy state without holes) lies in the odd N sector. Similar behaviour are also found for the open chain with diagonal boundary terms, for certain values of boundary parameters [47]. It is known that (critical) XXZ model with nondiagonal boundary terms corresponds to (conformally invariant) free Boson with Neumann boundary condition whereas the diagonal ones are related to the Dirichlet case [34 − 36, 42]. Although the model we study here has nondiagonal boundary terms, we find that the conformal dimensions for this model resemble that of the Dirichlet boundary condition. Some numerical results are presented in section 4 to confirm and support the analytical results derived in section 3. Here, we solve the model numerically for some large but finite N and further employ an algorithm due to Vanden Broeck and Schwartz [39]–[40] to extrapolate the results for $N \to \infty$ limit. We conclude with a discussion of our results and some potential open problems in section 5.

2. Bethe ansatz

We begin this section by reviewing recently proposed Bethe Ansatz solution [11, 38] for the following model [43, 44]

$$\mathcal{H} = \mathcal{H}_0 + \frac{1}{2} \sinh \eta (\operatorname{cosech} \alpha_- \sigma_1^x + \operatorname{cosech} \alpha_+ \sigma_N^x) , \tag{2.1}$$

[1] This solution, in contrast to [6]–[9] does not assume any constraint among the boundary parameters.

where the "bulk" Hamiltonian is given by

$$\mathcal{H}_0 = \frac{1}{2}\sum_{n=1}^{N-1}\left(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + \cosh\eta\ \sigma_n^z\sigma_{n+1}^z\right) . \tag{2.2}$$

In the above expressions, σ^x, σ^y, σ^z are the usual Pauli matrices, η is the bulk anisotropy parameter (taking values $\eta = \frac{i\pi}{p+1}$, with p odd), $\alpha_\pm$ are the boundary parameters, and N is the number of spins/sites. Note that, this model has only two boundary parameters. Other boundary parameters (as they appear in the original Hamiltonian in [43]) have been set to zero. We restrict the values of $\alpha_\pm$ to be pure imaginary to ensure the Hermiticity of the Hamiltonian. The Bethe Ansatz equations for both odd and even N are given by

$$\begin{aligned}\frac{\delta(u_j^{(1)})\ h^{(2)}(u_j^{(1)}-\eta)}{\delta(u_j^{(1)}-\eta)\ h^{(1)}(u_j^{(1)})} &= -\frac{Q_2(u_j^{(1)}-\eta)}{Q_2(u_j^{(1)}+\eta)}\,, \qquad j = 1\,,2\,,\ldots\,,M_1\,,\\ \frac{h^{(1)}(u_j^{(2)}-\eta)}{h^{(2)}(u_j^{(2)})} &= -\frac{Q_1(u_j^{(2)}+\eta)}{Q_1(u_j^{(2)}-\eta)}\,, \qquad j = 1\,,2\,,\ldots\,,M_2\,.\end{aligned} \tag{2.3}$$

where

$$\begin{aligned}\delta(u) \;=\; & 2^4\left(\sinh u \sinh(u+2\eta)\right)^{2N}\frac{\sinh 2u \sinh(2u+4\eta)}{\sinh(2u+\eta)\sinh(2u+3\eta)}\sinh(u+\eta+\alpha_-)\\ & \sinh(u+\eta-\alpha_-)\sinh(u+\eta+\alpha_+)\sinh(u+\eta-\alpha_+)\cosh^4(u+\eta)\end{aligned} \tag{2.4}$$

and

$$Q_a(u) = \prod_{j=1}^{M_a}\sinh(u-u_j^{(a)})\sinh(u+u_j^{(a)}+\eta)\,, \qquad a = 1\,,2\,, \tag{2.5}$$

M_1 and M_2 are the number of Bethe roots, $u_j^{(1)}$ and $u_j^{(2)}$ (zeros of $Q_1(u)$ and $Q_2(u)$ respectively). However, $h^{(1)}(u)$ and $h^{(2)}(u)$ differ for odd and even values of N, as will be noted below. The energy eigenvalues in terms of the "shifted" Bethe roots $\tilde{u}_j^{(a)}$ are given by

$$E = \frac{1}{2}\sinh^2\eta\sum_{a=1}^{2}\sum_{j=1}^{M_a}\frac{1}{\sinh\left(\tilde{u}_j^{(a)}-\frac{\eta}{2}\right)\sinh\left(\tilde{u}_j^{(a)}+\frac{\eta}{2}\right)} + \frac{1}{2}(N-1)\cosh\eta\,. \tag{2.6}$$

where $\tilde{u}_j^{(a)} \equiv u_j^{(a)} + \frac{\eta}{2}$.

2.1 Even N

We begin by recalling [38] the structure of roots distribution for this case. The Bethe roots $\tilde{u}_j^{(a)}$ for the lowest energy state have the form

$$\begin{cases} \mu\lambda_j^{(a,1)} & : \ j = 1\,,2\,,\ldots\,,M_{(a,1)} \\ \mu\lambda_j^{(a,2)} + \frac{i\pi}{2}\,, & : \ j = 1\,,2\,,\ldots\,,M_{(a,2)} \end{cases}\,, \qquad a = 1\,,2\,, \tag{2.7}$$

where $\lambda_j^{(a,b)}$ are real. Here, $M_{(1,1)} = M_{(2,1)} = \frac{N}{2}$, and $M_{(1,2)} = \frac{p+1}{2}$, $M_{(2,2)} = \frac{p-1}{2}$. The $\mu\lambda_j^{(a,1)}$ are the zeros of $Q_a(u)$ that form real sea ("sea roots") and $\mu\lambda_k^{(a,2)}$ are real parts of the "extra roots" (also zeros of $Q_a(u)$) which are not part of the "seas". Hence, there are two "seas" of real roots. We employ notations similar to the one used in [28],

$$e_n(\lambda) = \frac{\sinh\left(\mu(\lambda + \frac{in}{2})\right)}{\sinh\left(\mu(\lambda - \frac{in}{2})\right)}, \qquad g_n(\lambda) = e_n\left(\lambda \pm \frac{i\pi}{2\mu}\right) = \frac{\cosh\left(\mu(\lambda + \frac{in}{2})\right)}{\cosh\left(\mu(\lambda - \frac{in}{2})\right)}. \tag{2.8}$$

Rewriting bulk and boundary parameters [28], $\eta = i\mu$, $\alpha_\pm = i\mu a_\pm$,[2] where $\mu = \frac{\pi}{p+1}$ and taking

$$h^{(1)}(u) = \frac{8\sinh^{2N+1}(u+2\eta)\cosh^2(u+\eta)\cosh(u+2\eta)}{\sinh(2u+3\eta)}, \quad h^{(2)}(u) = h^{(1)}(-u-2\eta), \tag{2.9}$$

the Bethe Ansatz equations (2.3) for the sea roots then take the following form [11, 38]

$$\begin{aligned} e_1\left(\lambda_j^{(1,1)}\right)^{2N+1}&\left[g_1\left(\lambda_j^{(1,1)}\right)e_{1+2a_-}\left(\lambda_j^{(1,1)}\right)e_{1-2a_-}\left(\lambda_j^{(1,1)}\right)e_{1+2a_+}\left(\lambda_j^{(1,1)}\right)e_{1-2a_+}\left(\lambda_j^{(1,1)}\right)\right]^{-1} \\ = -\prod_{k=1}^{N/2}&\left[e_2\left(\lambda_j^{(1,1)}-\lambda_k^{(2,1)}\right)e_2\left(\lambda_j^{(1,1)}+\lambda_k^{(2,1)}\right)\right]\prod_{k=1}^{(p-1)/2}\left[g_2\left(\lambda_j^{(1,1)}-\lambda_k^{(2,2)}\right)g_2\left(\lambda_j^{(1,1)}+\lambda_k^{(2,2)}\right)\right], \end{aligned} \tag{2.10}$$

and

$$\begin{aligned} e_1\left(\lambda_j^{(2,1)}\right)^{2N+1} g_1\left(\lambda_j^{(2,1)}\right)^{-1} &= -\prod_{k=1}^{N/2}\left[e_2\left(\lambda_j^{(2,1)}-\lambda_k^{(1,1)}\right)e_2\left(\lambda_j^{(2,1)}+\lambda_k^{(1,1)}\right)\right]\times \\ &\times \prod_{k=1}^{(p+1)/2}\left[g_2\left(\lambda_j^{(2,1)}-\lambda_k^{(1,2)}\right)g_2\left(\lambda_j^{(2,1)}+\lambda_k^{(1,2)}\right)\right], \end{aligned} \tag{2.11}$$

respectively, where $j = 1, \ldots, \frac{N}{2}$. The corresponding ground-state counting functions are

$$\begin{aligned} \mathsf{h}^{(1)}(\lambda) = \frac{1}{2\pi}\Big\{&(2N+1)q_1(\lambda)-r_1(\lambda)-q_{1+2a_-}(\lambda)-q_{1-2a_-}(\lambda)-q_{1+2a_+}(\lambda)-q_{1-2a_+}(\lambda) \\ &-\sum_{k=1}^{N/2}\left[q_2\left(\lambda-\lambda_k^{(2,1)}\right)+q_2\left(\lambda+\lambda_k^{(2,1)}\right)\right]-\sum_{k=1}^{(p-1)/2}\left[r_2\left(\lambda-\lambda_k^{(2,2)}\right)+r_2\left(\lambda+\lambda_k^{(2,2)}\right)\right]\Big\}, \end{aligned} \tag{2.12}$$

and

$$\begin{aligned} \mathsf{h}^{(2)}(\lambda) = \frac{1}{2\pi}\Big\{&(2N+1)q_1(\lambda) - r_1(\lambda) - \sum_{k=1}^{N/2}\left[q_2\left(\lambda-\lambda_k^{(1,1)}\right)+q_2\left(\lambda+\lambda_k^{(1,1)}\right)\right] \\ &- \sum_{k=1}^{(p+1)/2}\left[r_2\left(\lambda-\lambda_k^{(1,2)}\right)+r_2\left(\lambda+\lambda_k^{(1,2)}\right)\right]\Big\}. \end{aligned} \tag{2.13}$$

[2]Bethe Ansatz equations written in this and subsequent sections are true only for suitable values of $a_\pm$, namely $\frac{\nu-1}{2} < |a_\pm| < \frac{\nu+1}{2}$, $\quad a_+a_- > 0$, where $\nu = p+1$

where $q_n(\lambda)$ and $r_n(\lambda)$ are odd functions defined by

$$
\begin{aligned}
q_n(\lambda) &= \pi + i \ln e_n(\lambda) = 2\tan^{-1}\left(\cot(n\mu/2)\tanh(\mu\lambda)\right) , \\
r_n(\lambda) &= i \ln g_n(\lambda) .
\end{aligned} \tag{2.14}
$$

These counting functions satisfy the following

$$
\mathsf{h}^{(l)}(\lambda_j) = j , \qquad j = 1 , \dots , \frac{N}{2} \tag{2.15}
$$

In (2.15) above, $l = 1 , 2$

2.2 Odd N

In this section, we present an extension of the previous results to include solutions for odd N values. The roots distribution is similar to the previous case, but now we have $M_{(1,1)} = M_{(2,1)} = \frac{N+1}{2}$, and $M_{(1,2)} = M_{(2,2)} = \frac{p-1}{2}$. Using the following in (2.3),

$$
\begin{aligned}
h^{(1)}(u) &= \frac{\sinh(u - \alpha_+ + \eta)\sinh(u + \alpha_+ + \eta)\sinh^{2N+1}(u + 2\eta)\cosh^2(u + \eta)\cosh(u + 2\eta)}{\sinh(2u + 3\eta)} , \\
h^{(2)}(u) &= h^{(1)}(-u - 2\eta) ,
\end{aligned} \tag{2.16}
$$

we obtain the Bethe Ansatz equations

$$
\begin{aligned}
&e_1\left(\lambda_j^{(1,1)}\right)^{2N+1}\left[g_1\left(\lambda_j^{(1,1)}\right)e_{1+2a_-}\left(\lambda_j^{(1,1)}\right)e_{1-2a_-}\left(\lambda_j^{(1,1)}\right)\right]^{-1} = \\
&-\prod_{k=1}^{(N+1)/2}\left[e_2\left(\lambda_j^{(1,1)}-\lambda_k^{(2,1)}\right)e_2\left(\lambda_j^{(1,1)}+\lambda_k^{(2,1)}\right)\right]\prod_{k=1}^{(p-1)/2}\left[g_2\left(\lambda_j^{(1,1)}-\lambda_k^{(2,2)}\right)g_2\left(\lambda_j^{(1,1)}+\lambda_k^{(2,2)}\right)\right] ,
\end{aligned} \tag{2.17}
$$

and

$$
\begin{aligned}
&e_1\left(\lambda_j^{(2,1)}\right)^{2N+1}\left[g_1\left(\lambda_j^{(2,1)}\right)e_{1+2a_+}\left(\lambda_j^{(2,1)}\right)e_{1-2a_+}\left(\lambda_j^{(2,1)}\right)\right]^{-1} = \\
&-\prod_{k=1}^{(N+1)/2}\left[e_2\left(\lambda_j^{(2,1)}-\lambda_k^{(1,1)}\right)e_2\left(\lambda_j^{(2,1)}+\lambda_k^{(1,1)}\right)\right]\prod_{k=1}^{(p-1)/2}\left[g_2\left(\lambda_j^{(2,1)}-\lambda_k^{(1,2)}\right)g_2\left(\lambda_j^{(2,1)}+\lambda_k^{(1,2)}\right)\right] ,
\end{aligned} \tag{2.18}
$$

respectively, where $j = 1 , \dots , \frac{N+1}{2}$. Note the presence of parameter-dependant terms in both the equations above. One can also notice the number of extra roots changes from $\frac{p+1}{2}$ to $\frac{p-1}{2}$ for $Q_1(u)$. The ground-state counting functions for this case read

$$
\begin{aligned}
\mathsf{h}^{(1)}(\lambda) = \frac{1}{2\pi}\Bigg\{&(2N+1)q_1(\lambda)-r_1(\lambda)-q_{1+2a_-}(\lambda)-q_{1-2a_-}(\lambda) \\
&-\sum_{k=1}^{(N+1)/2}\left[q_2\left(\lambda-\lambda_k^{(2,1)}\right)+q_2\left(\lambda+\lambda_k^{(2,1)}\right)\right]-\sum_{k=1}^{(p-1)/2}\left[r_2\left(\lambda-\lambda_k^{(2,2)}\right)+r_2\left(\lambda+\lambda_k^{(2,2)}\right)\right]\Bigg\} ,
\end{aligned} \tag{2.19}
$$

and

$$
\begin{aligned}
\mathsf{h}^{(2)}(\lambda) = \frac{1}{2\pi}\Bigg\{&(2N+1)q_1(\lambda)-r_1(\lambda)-q_{1+2a_+}(\lambda)-q_{1-2a_+}(\lambda) \\
&-\sum_{k=1}^{(N+1)/2}\left[q_2\left(\lambda-\lambda_k^{(1,1)}\right)+q_2\left(\lambda+\lambda_k^{(1,1)}\right)\right]-\sum_{k=1}^{(p-1)/2}\left[r_2\left(\lambda-\lambda_k^{(1,2)}\right)+r_2\left(\lambda+\lambda_k^{(1,2)}\right)\right]\Bigg\} ,
\end{aligned} \tag{2.20}
$$

As for even N, we again have the following

$$\mathsf{h}^{(l)}(\lambda_j) = j\,, \qquad j = 1\,, \dots\,, \frac{N+1}{2} \tag{2.21}$$

where $l = 1\,, 2$. Note that (2.15) and (2.21) can be written more compactly as

$$\mathsf{h}^{(l)}(\lambda_j) = j\,, \qquad j = 1\,, \dots\,, \left\lfloor \frac{N+1}{2} \right\rfloor \tag{2.22}$$

where $\lfloor \dots \rfloor$ denotes the integer part and $\mu\lambda_{\lfloor \frac{N+1}{2} \rfloor}$ is the largest sea root for that "sea". Subsequently, we shall denote largest sea roots as $\mu\Lambda_l$.

3. Finite-size correction of order $1/N$

In this section, we shall compute the finite-size correction for the ground state and low lying excited states. For these excited states, we restrict our analysis to excitations by holes which are located to the right of the real sea roots. Applying (2.7) to (2.6), we get the lowest state energy eigenvalues for chain of finite length N,

$$E = -\frac{\pi \sin\mu}{\mu} \left\{ \frac{1}{2} \sum_{a=1}^{2} \sum_{j=-\lfloor \frac{N+1}{2} \rfloor}^{\lfloor \frac{N+1}{2} \rfloor} a_1\left(\lambda_j^{(a,1)}\right) - a_1(0) + \sum_{a=1}^{2} \sum_{j=1}^{M_{(a,2)}} b_1\left(\lambda_j^{(a,2)}\right) \right\} + \frac{1}{2}(N-1)\cos\mu\,. \tag{3.1}$$

where notations from [28] have again been adopted

$$\begin{aligned} a_n(\lambda) &= \frac{1}{2\pi}\frac{d}{d\lambda} q_n(\lambda) = \frac{\mu}{\pi} \frac{\sin(n\mu)}{\cosh(2\mu\lambda) - \cos(n\mu)}\,, \\ b_n(\lambda) &= \frac{1}{2\pi}\frac{d}{d\lambda} r_n(\lambda) = -\frac{\mu}{\pi} \frac{\sin(n\mu)}{\cosh(2\mu\lambda) + \cos(n\mu)}\,. \end{aligned} \tag{3.2}$$

Note that $M_{(a,2)}$ in (3.1), refers to number of extra roots for $Q_a(u)$. The first and third terms in the curly bracket of (3.1) are summed over the number of sea roots and extra roots respectively. As one considers next lowest excited state, the number of sea roots and extra roots change. Hence, for these states of low lying excitations (with real sea), the very same term in the first sum will again be summed over accordingly between approriate limits dictated by the number of sea roots. As for the summation over extra roots, the function summed over depends on the imaginary part of these roots, especially in the presence of 2-strings. However, as one shall see, for $1/N$ correction (in the $N \to \infty$ limit), only the sum over the sea roots contributes. The second sum in (3.1) contributes to order 1 correction (boundary energy) which we have considered elsewhere[3][38].

[3]Equation (4.26) for the boundary energy in [38] holds both for even and odd values of N

JHEP05(2007)069

3.1 Sum-rule and hole-excitations

Now we present some results based on the solution of the model (2.1) for $N = 2\,,3\,,\ldots\,,7$. We begin with even N case. We find for even N, excited states contain odd number of holes for each $Q_a(u)$. This can be seen from the following analysis on counting functions. For the lowest energy state the counting functions are given by (2.12) and (2.13). By using the fact that $q_n(\lambda) \to \mathrm{sgn}(n)\pi - \mu n$ and $r_n(\lambda) \to -\mu n$ as $\lambda \to \infty$ and $\rho^{(l)} = \frac{1}{N}\frac{d\mathsf{h}^{(l)}}{d\lambda}$ we have the following sum rule

$$\begin{aligned}\int_{\Lambda_l}^{\infty} d\lambda\ \rho^{(l)}(\lambda) &= \frac{1}{N}\Big(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)\Big)\\ &= \frac{1}{N}\left(\frac{1}{2}+1\right)\end{aligned} \tag{3.3}$$

$\mu\Lambda_l$ refers to the largest sea root. As before $l = 1\,,2$. We make use of the fact that

$$\begin{aligned}\mathsf{h}^{(l)}(\infty) &= \frac{N}{2}+\frac{3}{2}\\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N}{2}\end{aligned} \tag{3.4}$$

From (3.3) and (3.4), we see that there is one hole located to the right of the largest sea root. Similar analysis for low lying (multi-hole) excited states yields the following

$$\begin{aligned}\int_{\Lambda_l}^{\infty} d\lambda\ \rho^{(l)}(\lambda) &= \frac{1}{N}\Big(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)\Big)\\ &= \frac{1}{N}\left(\frac{1}{2}+N_H\right)\end{aligned} \tag{3.5}$$

where N_H is the number of holes (odd) to the right of the corresponding largest sea root. To illustrate the results above, we consider the following low lying excited states with $\frac{N}{2}-1$ and $\frac{N}{2}-2$ sea roots and therefore different number of extra roots than the lowest energy state.[4] The former case is found to have one hole with $\frac{p-1}{2}$ and $\frac{p-3}{2}$ extra roots in addition to a 2-string from each of the $Q_1(u)$ and $Q_2(u)$ respectively. From,

$$\begin{aligned}\mathsf{h}^{(l)}(\infty) &= \frac{N}{2}+\frac{1}{2}\\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N}{2}-1\end{aligned} \tag{3.6}$$

one has

$$\frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) = \frac{1}{N}\left(\frac{1}{2}+1\right) \tag{3.7}$$

Hence giving $N_H = 1$. The later case has three holes with $\frac{p+1}{2}$ and $\frac{p-1}{2}$ extra roots and a 2-string from each of the $Q_a(u)$ with $a = 1\,,2$. Similar analysis,

$$\begin{aligned}\mathsf{h}^{(l)}(\infty) &= \frac{N}{2}+\frac{3}{2}\\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N}{2}-2\end{aligned} \tag{3.8}$$

[4] The lowest energy state has $\frac{N}{2}$ sea roots. As for the extra roots, there are $\frac{p+1}{2}$ and $\frac{p-1}{2}$ of them for $Q_1(u)$ and $Q_2(u)$ respectively

yields

$$\frac{1}{N}(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)) = \frac{1}{N}\left(\frac{1}{2} + 3\right) \tag{3.9}$$

giving $N_H = 3$. The total number of roots are the same for all these states. There are also excited states with equal number of sea and extra roots as for the state of lowest energy, but with position of the single hole nearer to the origin than that of the lowest energy state, suggesting the usual bulk hole-excitation scenario, $E_{\text{hole}}(\lambda^{(a)})$ increases as $\lambda^{(a)} \to 0$ where $E_{\text{hole}}(\lambda^{(a)})$ is the energy due to the presence of holes and $\lambda^{(a)}$, with $a = 1\,,2$ denote the positions of the holes in both "seas". We shall compute the explicit expression for energy due to holes shortly.

As for the odd N case, we have the true ground state, namely state of lowest energy without hole. From the counting functions, (2.19) and (2.20), we have

$$\int_{\Lambda_l}^{\infty} d\lambda\ \rho^{(l)}(\lambda) = \frac{1}{N}\Big(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)\Big) = \frac{1}{2N} \tag{3.10}$$

As before $l = 1\,,2$, and we make use of the fact that

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) &= \frac{N}{2} + 1 \\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N+1}{2} \end{aligned} \tag{3.11}$$

From (3.11), we see that this state of lowest energy for odd N has no hole, signifying the true ground state. Similar analysis for low lying excited states yields the following

$$\begin{aligned} \int_{\Lambda_l}^{\infty} d\lambda\ \rho^{(l)}(\lambda) &= \frac{1}{N}\Big(\mathsf{h}^{(l)}(\infty) - \mathsf{h}^{(l)}(\Lambda_l)\Big) \\ &= \frac{1}{N}\left(\frac{1}{2} + N_H\right) \end{aligned} \tag{3.12}$$

where N_H is the number of holes (even) to the right of sea roots. Hence, for odd N case, there are even number of holes (for each $Q_a(u)$), with $a = 1\,,2$, for the excited states, e.g., for the first excited state with $\frac{N-1}{2}$ sea roots,

$$\begin{aligned} \mathsf{h}^{(l)}(\infty) &= \frac{N+1}{2} + \frac{3}{2} \\ \mathsf{h}^{(l)}(\Lambda_l) &= \frac{N-1}{2} \end{aligned} \tag{3.13}$$

which signifies the presence of two holes.

It is known for simpler models of spin chains e.g., closed XXZ chain that even number of holes are present in chains with even number of spins and vice versa. Hence, the true ground state (lowest energy state with no holes) for these models is found to lie in even N sector. The reverse scenario (one hole in the lowest energy state for even N and ground state in odd N sector) we find here for this model can be explained using some heuristic arguments based on spin and magnetic fields at the two boundaries, similar to the one given in section 3 of [38].[5] In footnote 2, we notice the signs of a_+ and a_- must be the same for boundary parameter region of interest. Hence, in Hamiltonian (2.1), the direction of the magnetic fields at the two boundaries are also the same (Both up or both down). This upsets the antiferromagnetic spin arrangement at the boundaries, favouring spin allignments along the same direction at the boundaries for chains with even N. This causes the following: presence of odd N behaviours in the even N chain, namely the lowest energy state for even N sector has one hole for each $Q_a(u)$. Spins at the boundaries for the odd N chain will not experience such spin upset since the parallel magnetic fields favours the antiferromagnetic arrangement of an odd N chain. Therefore, the lowest energy state for odd N chain has no holes. In other words, the true ground state exists in odd N sector. Further effects are the presence of odd and even number of holes in chains with even and odd N respectively as shown in the analysis above.

Now, the energy due to hole excitations can be presented. We consider first the lowest energy state for even N case with one hole. Using

$$\frac{1}{N}\sum_{k=-\frac{N}{2}}^{\frac{N}{2}} g(\lambda-\lambda_k^{(a,1)}) \approx \int_{-\infty}^{\infty} d\lambda'\ \rho^{(l)}(\lambda')g(\lambda-\lambda') - \frac{1}{N}g(\lambda-\tilde{\lambda}^{(a)}) \tag{3.14}$$

for some arbitrary function $g(\lambda)$ and

$$\rho^{(l)} = \frac{1}{N}\frac{d\mathsf{h}^{(l)}}{d\lambda} \tag{3.15}$$

where $l = 1\,,2$, $\mu\lambda_k^{(a,1)} \equiv$ sea roots, with $a = 1\,,2$, and $\mu\tilde{\lambda}^{(a)} \equiv$ position of the hole for each of the $Q_a(u)$, one can write down the sum of the two densities

$$\begin{aligned}
\rho^{(1)}(\lambda)+\rho^{(2)}(\lambda) =& 4a_1(\lambda) - \int_{-\infty}^{\infty} d\lambda'(\rho^{(1)}(\lambda')+\rho^{(2)}(\lambda'))a_2(\lambda-\lambda') + \frac{1}{N}\Big[a_2(\lambda-\tilde{\lambda}^{(1)})+a_2(\lambda-\tilde{\lambda}^{(2)})\Big] \\
&+\frac{1}{N}\Big[2a_1(\lambda)+2a_2(\lambda)-2b_1(\lambda)-a_{1+2a_-}(\lambda)-a_{1-2a_-}(\lambda)-a_{1+2a_+}(\lambda)-a_{1-2a_+}(\lambda) \\
&-\sum_{k=1}^{\frac{p-1}{2}}\left(b_2\left(\lambda-\lambda_k^{(2,2)}\right)+b_2\left(\lambda+\lambda_k^{(2,2)}\right)\right) \\
&-\sum_{k=1}^{\frac{p+1}{2}}\left(b_2\left(\lambda-\lambda_k^{(1,2)}\right)+b_2\left(\lambda+\lambda_k^{(1,2)}\right)\right)\Big]
\end{aligned} \tag{3.16}$$

Defining $\rho_{\text{total}}(\lambda) \equiv \rho^{(1)}(\lambda) + \rho^{(2)}(\lambda)$ and solving (3.16) using Fourier transform,[6] we have

$$\hat{\rho}_{\text{total}}(\omega) = 4\hat{s}(\omega) + \frac{1}{N}\hat{R}(\omega) + \frac{1}{N}\hat{J}(\omega)\left(e^{i\omega\tilde{\lambda}^{(1)}} + e^{i\omega\tilde{\lambda}^{(2)}}\right) \tag{3.17}$$

where $\hat{\rho}_{\text{total}}(\omega)\,, \hat{a}_2(\omega)$[7] and $\hat{s}(\omega)$ are the Fourier transforms of $\rho_{\text{total}}(\lambda)\,, a_2(\lambda)$ and $\frac{a_1(\lambda)}{1+a_2(\lambda)}$

[5] Readers are urged to refer to figures 2 and 3 in that section

[6] Our conventions are

$$\hat{f}(\omega) \equiv \int_{-\infty}^{\infty} e^{i\omega\lambda}\ f(\lambda)\ d\lambda\,, \qquad f(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega\lambda}\ \hat{f}(\omega)\ d\omega\,.$$

[7] $\hat{a}_n(\omega) = \text{sgn}(n)\frac{\sinh((\nu-|n|)\omega/2)}{\sinh(\nu\omega/2)}\,, \qquad 0 \le |n| < 2\nu\,.$

respectively. Also $\hat{J}(\omega) = \frac{\hat{a}_2(\omega)}{1+\hat{a}_2(\omega)}$. $\hat{R}(\omega)$ is the contribution from the second square bracket in (3.16), which will not enter the calculation for $E_{\text{hole}}(\tilde{\lambda}^{(a)})$ and will be omitted henceforth. The Fourier transform of hole density are the third and the fourth terms in (3.17), which gives

$$\rho_{\text{hole}}(\lambda) = \frac{1}{N}\Big[J(\lambda - \tilde{\lambda}^{(1)}) + J(\lambda - \tilde{\lambda}^{(2)})\Big] \tag{3.18}$$

Using approximation (3.14) in (3.1), and making use of (3.18), one has

$$E_{\text{hole}}(\tilde{\lambda}^{(a)}) = -\frac{N\pi\sin\mu}{2\mu}\int_{-\infty}^{\infty} d\lambda\ a_1(\lambda)\rho_{\text{hole}}(\lambda) + \frac{\pi\sin\mu}{2\mu}\sum_{a=1}^{2} a_1(\tilde{\lambda}^{(a)}) \tag{3.19}$$

which after some manipulation yields

$$E_{\text{hole}}(\tilde{\lambda}^{(a)}) = \frac{\pi\sin\mu}{4\mu}\sum_{a=1}^{2}\frac{1}{\cosh\pi\tilde{\lambda}^{(a)}} \tag{3.20}$$

Generalizing the derivation to α number of holes, one has

$$\rho_{\text{hole}}(\lambda) = \frac{1}{N}\sum_{\alpha}\sum_{a=1}^{2} J(\lambda - \tilde{\lambda}_{\alpha}^{(a)}) \tag{3.21}$$

and finally the following for the energy

$$E_{\text{hole}}(\tilde{\lambda}_{\alpha}^{(a)}) = \frac{\pi\sin\mu}{4\mu}\sum_{\alpha}\sum_{a=1}^{2}\frac{1}{\cosh\pi\tilde{\lambda}_{\alpha}^{(a)}} \tag{3.22}$$

Note that $E_{\text{hole}}(\tilde{\lambda}_{\alpha}^{(a)})$ increases as $\tilde{\lambda}_{\alpha}^{(a)} \to 0$ as mentioned above in paragraph following (3.9).

3.2 Casimir energy

In this section, we give the derivation of $1/N$ correction (Casimir energy) to the lowest energy state, for the even N case (with one hole). This result is then generalized to include odd N values as well as the low lying (multi-hole) excited states. We begin by presenting the expression for the density difference between chain of finite length (with N spins), $\rho_N^{(1)}(\lambda) + \rho_N^{(2)}(\lambda)$ and that of infinite length, $\rho_\infty(\lambda)$

$$\begin{aligned}
\rho_N^{(1)}(\lambda) + \rho_N^{(2)}(\lambda) - \rho_\infty(\lambda) = &-\int_{-\infty}^{\infty} d\gamma\ a_2(\lambda-\gamma)\Bigg[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta\Big(\gamma - \lambda_\beta^{(1,1)}\Big) - \rho_N^{(1)}(\gamma)\Bigg] \\
&-\int_{-\infty}^{\infty} d\gamma\ a_2(\lambda-\gamma)\Bigg[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta\Big(\gamma - \lambda_\beta^{(2,1)}\Big) - \rho_N^{(2)}(\gamma)\Bigg] \\
&-\int_{-\infty}^{\infty} d\gamma\ a_2(\lambda-\gamma)\Big[\rho_N^{(1)}(\gamma) + \rho_N^{(2)}(\gamma) - \rho_\infty(\gamma)\Big]
\end{aligned} \tag{3.23}$$

In (3.23) and henceforth, only terms that are crucial to the computation of $1/N$ correction are given. Other parameter dependant terms that contribute to order 1 correction have been omitted here.[8] Solving (3.23) yields

$$\begin{aligned}\rho_N^{(1)}(\lambda)+\rho_N^{(2)}(\lambda)-\rho_\infty(\lambda) &= -\int_{-\infty}^{\infty} d\gamma\; p(\lambda-\gamma)\Big[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta\Big(\gamma-\lambda_\beta^{(1,1)}\Big)-\rho_N^{(1)}(\gamma)\Big]\\ &\quad -\int_{-\infty}^{\infty} d\gamma\; p(\lambda-\gamma)\Big[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta\Big(\gamma-\lambda_\beta^{(2,1)}\Big)-\rho_N^{(2)}(\gamma)\Big] \qquad (3.24)\end{aligned}$$

where $\rho_\infty(\lambda)=\frac{4a_1(\lambda)}{1+a_2(\lambda)}\equiv 4s(\lambda)$ and $p(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\; e^{-i\omega\lambda}\frac{\hat{a}_2(\omega)}{1+\hat{a}_2(\omega)}$ Similar equation expressing the energy difference between finite and infinite system is also needed to compute Casimir energy. This is given by

$$\begin{aligned}E_N-E_\infty &= -\frac{N\pi\sin\mu}{2\mu}\Big\{\int_{-\infty}^{\infty}d\lambda\; a_1(\lambda)\Big[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta\Big(\lambda-\lambda_\beta^{(1,1)}\Big)-\rho_N^{(1)}(\lambda)\Big]\\ &\quad +\int_{-\infty}^{\infty}d\lambda\; a_1(\lambda)\Big[\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta\Big(\lambda-\lambda_\beta^{(2,1)}\Big)-\rho_N^{(2)}(\lambda)\Big]\\ &\quad +\int_{-\infty}^{\infty}d\lambda\; a_1(\lambda)\Big[\rho_N^{(1)}(\lambda)+\rho_N^{(2)}(\lambda)-\rho_\infty(\lambda)\Big]\Big\} \qquad (3.25)\end{aligned}$$

Using (3.24) and the fact that $\hat{p}(\omega)\hat{a}_1(\omega)=\hat{s}(\omega)\hat{a}_2(\omega)$, we have

$$E_N-E_\infty = -\frac{N\pi\sin\mu}{4\mu}\Big\{\int_{-\infty}^{\infty}d\lambda\; S_N^{(1)}(\lambda)\rho_\infty^{(1)}(\lambda)+\int_{-\infty}^{\infty}d\lambda\; S_N^{(2)}(\lambda)\rho_\infty^{(2)}(\lambda)\Big\} \qquad (3.26)$$

where $S_N^{(l)}(\lambda)\equiv\frac{1}{N}\sum_{\beta=-\frac{N}{2}}^{\frac{N}{2}}\delta(\lambda-\lambda_\beta^{(l,1)})-\rho_N^{(l)}(\lambda)$ and $\rho_\infty^{(l)}(\lambda)=\frac{1}{2}\rho_\infty(\lambda)\equiv 2s(\lambda)$ with $l=1\,,2$. Further, using Euler-Maclaurin summation formula [45], (3.26) becomes

$$\begin{aligned}E_N-E_\infty &= -\frac{N\pi\sin\mu}{2\mu}\Big\{-\int_{\Lambda_1}^{\infty}d\lambda\; \rho_\infty^{(1)}(\lambda)\rho_N^{(1)}(\lambda)+\frac{1}{2N}\rho_\infty^{(1)}(\Lambda_1)+\frac{1}{12N^2\rho_N^{(1)}(\Lambda_1)}\rho_\infty^{(1)\prime}(\Lambda_1)\\ &\quad -\int_{\Lambda_2}^{\infty}d\lambda\; \rho_\infty^{(2)}(\lambda)\rho_N^{(2)}(\lambda)+\frac{1}{2N}\rho_\infty^{(2)}(\Lambda_2)+\frac{1}{12N^2\rho_N^{(2)}(\Lambda_2)}\rho_\infty^{(2)\prime}(\Lambda_2)\Big\} \qquad (3.27)\end{aligned}$$

(3.24) can also be expressed in similar form

$$\begin{aligned}\rho_N^{(1)}(\lambda)+\rho_N^{(2)}(\lambda)-\rho_\infty(\lambda) &= \int_{\Lambda_1}^{\infty}d\gamma p(\lambda-\gamma)\rho_N^{(1)}(\gamma)-\frac{1}{2N}p(\lambda-\Lambda_1)-\frac{p'(\lambda-\Lambda_1)}{12N^2\rho_N^{(1)}(\Lambda_1)}\\ &\quad +\int_{\Lambda_2}^{\infty}d\gamma p(\lambda-\gamma)\rho_N^{(2)}(\gamma)-\frac{1}{2N}p(\lambda-\Lambda_2)-\frac{p'(\lambda-\Lambda_2)}{12N^2\rho_N^{(2)}(\Lambda_2)} \qquad (3.28)\end{aligned}$$

[8] See [38] for details

As before, $\mu\Lambda_1$ and $\mu\Lambda_2$ are the largest sea roots from the two "seas" respectively. From this point, the calculation very closely resembles the details found in section 2 in [3]. Hence, we omit the details and give only the crucial steps. Note that (3.28) can be written in the standard form of the Wiener-Hopf equation [46] after redefining the terms,

$$\begin{aligned}\chi^{(1)}(t)+\chi^{(2)}(t)-\int_0^{\infty}ds\ p(t-s)\chi^{(1)}(s)-\int_0^{\infty}ds\ p(t-s)\chi^{(2)}(s)\\ \approx f^{(1)}(t)-\frac{1}{2N}p(t)+\frac{1}{12N^2\rho_N^{(1)}(\Lambda_1)}p^{'}(t)+f^{(2)}(t)-\frac{1}{2N}p(t)+\frac{1}{12N^2\rho_N^{(2)}(\Lambda_2)}p^{'}(t)\end{aligned} \tag{3.29}$$

where the following definitions have been adopted

$$\begin{aligned}\chi^{(l)}(\lambda)&=\rho_N^{(l)}(\lambda+\Lambda_l)\\ f^{(l)}(\lambda)&=\rho_\infty^{(l)}(\lambda+\Lambda_l)\end{aligned} \tag{3.30}$$

and following change in variable is used: $t=\lambda-\Lambda_l$ with $l=1,2$ From the Fourier transformed version of (3.29), one can solve for $X_+^{(l)}(\omega)$ which is the Fourier transform of $\chi_+^{(l)}(t)$ that is analytic in the upper half complex plane,[9]

$$\begin{aligned}\hat{X}_+^{(l)}(\omega)=\frac{1}{2N}+\frac{i\omega}{12N^2\rho_N^{(l)}(\Lambda_l)}+G_+(\omega)\Bigg[&\frac{ig_1}{12N^2\rho_N^{(l)}(\Lambda_l)}-\frac{1}{2N}-\frac{i\omega}{12N^2\rho_N^{(l)}(\Lambda_l)}\\ &+\frac{\pi}{\pi-i\omega}\left(\frac{\alpha}{N}+\frac{1}{2N}-\frac{ig_1}{12N^2\rho_N^{(l)}(\Lambda_l)}\right)\Bigg]\end{aligned} \tag{3.31}$$

where $G_+(\omega)G_+(-\omega)=1+\hat{a}_2(\omega)$, $g_1=\frac{i}{12}(2+\nu-\frac{2\nu}{\nu-1})$ and $\alpha=\frac{1}{G_+(0)}=(\frac{\nu}{2(\nu-1)})^{\frac{1}{2}}$, with $G_+(0)^2=\frac{2(\nu-1)}{\nu}$. From (3.3), (3.30) and (3.31), one can then determine $\rho_N^{(1)}(\Lambda_1)$ and $\rho_N^{(2)}(\Lambda_2)$ explicitly from

$$\chi_+^{(l)}(0)\equiv\frac{1}{2}\rho_N^{(l)}(\Lambda_l)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\ \hat{X}_+^{(l)}(\omega) \tag{3.32}$$

by contour integration and some algebra. We give the result below

$$\rho_N^{(l)}(\Lambda_l)=\frac{1}{4N}\left\{\pi+2\pi\alpha+ig_1+\left[\pi^2+\frac{2ig_1\pi}{3}-\frac{g_1^2}{3}+4\pi^2\alpha^2+4\pi\alpha(\pi+ig_1)\right]^{\frac{1}{2}}\right\}. \tag{3.33}$$

Finally, using $\rho_\infty^{(l)}(\lambda)\approx 2e^{-\pi\lambda}$ for $\lambda\to\Lambda_l$ and (3.27), one arrives at the desired expression for $1/N$ correction to the energy,

$$E_N-E_\infty=E_{\text{Casimir}}=-\frac{\pi^2\sin\mu}{24\mu N}(1-12\alpha^2) \tag{3.34}$$

where the effective central charge is

$$c_{\text{eff}}=1-12\alpha^2=1-6\frac{\nu}{(\nu-1)} \tag{3.35}$$

[9] Again for complete details, refer to [3]

We see that for this model, the central charge, $c = 1$ (Free boson). Also c_{eff} is independent of boundary parameters, unlike for the Dirichlet case [3]. This is a feature expected for models with Neumann boundary condition. Further, from conformal field theory, one also has the following for the conformal dimensions,

$$\Delta = \frac{1 - c_{\mathrm{eff}}}{24} = \frac{\nu}{4(\nu - 1)} \tag{3.36}$$

Note that the above results are derived for the lowest energy state for even N with one hole for each $Q_a(u)$. Reviewing the derivation above, one can notice that the results above can be further generalized for any N and for low lying excited states with arbitrary number of holes, provided these holes are located to the right of the largest sea root as mentioned in the beginning of section 3. For these excited states, the sum for $S_N^{(l)}(\lambda)$ in (3.23) - (3.26) will inevitably have different limits since the number of sea roots vary. However, after applying the Euler-Maclaurin formula, one would recover (3.27) and (3.28). In addition to that, for states with N_H number of holes (all located to the right of the largest sea root), one uses the more general result for the sum rule, namely (3.5) and (3.12) which eventually yields

$$\alpha = \frac{N_H}{G_+(0)} \tag{3.37}$$

Thus, we have the following for the effective central charge and conformal dimensions for low lying excited states

$$\begin{aligned} c_{\mathrm{eff}} &= 1 - 6\frac{\nu}{(\nu - 1)} N_H^2 \\ \Delta &= \frac{\nu}{4(\nu - 1)} N_H^2 \end{aligned} \tag{3.38}$$

Surprisingly, the results (3.36) and (3.38) appear to have more resemblance to spin chains with diagonal boundary terms, as one could see from the $\frac{\nu}{\nu-1}$ dependance [33]–[36], rather than $\frac{\nu-1}{\nu}$ [42] which is the anticipated form for conformal dimensions for spin chains with nondiagonal boundary terms. Indeed the theory of a free Bosonic field φ compactified on a circle of radius r is invariant under $\varphi \mapsto \varphi + 2\pi r$, where $r = \frac{2}{\beta}$. β is the continuum bulk coupling constant that is related to ν by $\beta^2 = 8\pi(\frac{\nu-1}{\nu})$. Further, the quantization of the momentum zero-mode Π_0, yields $\Pi_0 = \frac{n\beta}{2}$ for Neumann boundary condition and $\Pi_0 = \frac{2n}{\beta}$ for the Dirichlet case, where n is an integer. Hence, the zero-mode contribution to the energy, $E_{0,n} \sim \Pi_0^2$ implies $E_{0,n} \sim \Delta \sim (\frac{\nu-1}{\nu})$ for Neumann and $E_{0,n} \sim \Delta \sim (\frac{\nu}{\nu-1})$ for Dirichlet case respectively. More complete discussion on this topic can be found in [35, 42]. Next, we will resort to numerical analysis to confirm our analytical results obtained in this section.

4. Numerical results

We present here some numerical results for both odd and even N cases, to support our analytical derivations in section 3.2. We first solve numerically the Bethe equations (2.3), (2.12), (2.13), (2.19) and (2.20) for some large number of spins. We use these

N	$c_{\text{eff}}\,, p=1\,,\nu=2$	$c_{\text{eff}}\,, p=3\,,\nu=4$
16	-9.365620	-2.853872
24	-9.857713	-3.271279
32	-10.122128	-3.557148
40	-10.287160	-3.770882
48	-10.399970	-3.939554
56	-10.481956	-4.077652
64	-10.544233	-4.193784
$\vdots$	$\vdots$	$\vdots$
∞	-11.000315	-7.000410

Table 1: Central charge values, c_{eff} for $p = 1$ ($a_+ = 0.783$, $a_- = 0.859$) and $p = 3$ ($a_+ = 2.29$, $a_- = 1.76$), from numerical computations based on $N = 16\,,24\,,\ldots\,,64$ and extrapolated values at $N \to \infty$ limit (Vanden Broeck and Schwartz algorithm).

solutions to calculate Casimir energy numerically from the following

$$E = E_{\text{bulk}} + E_{\text{boundary}} + E_{\text{Casimir}} \tag{4.1}$$

In (4.1), E is given by (3.1). Thus, having determined the Bethe roots numerically, one uses known expressions for E_{bulk} [48] and E_{boundary} [38] to determine E_{Casimir}. Then using the expression found above for E_{Casimir}, namely (3.34), one can determine the effective central charge, c_{eff} for that value of N,

$$c_{\text{eff}} = -\frac{24\mu N}{\pi^2 \sin\mu}(E - E_{\text{bulk}} - E_{\text{boundary}}) \tag{4.2}$$

Finally, we employ an algorithm due to Vanden Broeck and Schwartz [39]–[40] to extrapolate these values for central charge at $N \to \infty$ limit. Table 1 above shows the c_{eff} values for some finite even N, for the lowest energy state with one hole ($N_H = 1$). Equation (3.38) predicts c_{eff} values of -11 and -7 for $p = 1$ and $p = 3$[10] respectively which are the extrapolated values (-11.000315 and -7.000410) we obtain from the Vanden Broeck and Schwartz method.

For odd N sector, since $N_H = 0$, (3.38) predicts $c_{\text{eff}} = 1$ (for the ground state) for any odd p. We present similar numerical results for odd N in table 2 below for $p = 1$ and $p = 3$. We work out the c_{eff} values numerically for $N = 15\,,25\,,\ldots\,,65$. Excellent agreement between the calculated and the extrapolated values of 1.000770 and 1.001851 again strongly supports our analytical results.

5. Discussion

From the proposed Bethe ansatz equations for an open XXZ spin chain with special non-diagonal boundary terms at roots of unity, we computed finite size effect, namely the $1/N$

[10] $\nu = p + 1$

N	$c_{\rm eff}\,,\, p = 1\,, \nu = 2$	$c_{\rm eff}\,,\, p = 3\,, \nu = 4$
15	0.898334	0.531501
25	0.936128	0.634012
35	0.953433	0.692758
45	0.963360	0.731841
55	0.969797	0.760142
65	0.974311	0.781795
$\vdots$	$\vdots$	$\vdots$
∞	1.000770	1.001851

Table 2: Central charge values, $c_{\rm eff}$ for $p = 1$ ($a_+ = 0.926$, $a_- = 0.654$) and $p = 3$ ($a_+ = 2.10$, $a_- = 1.80$), from numerical computations based on $N = 15\,, 25\,, \ldots\,, 65$ and extrapolated values at $N \to \infty$ limit (Vanden Broeck and Schwartz algorithm).

correction (Casimir energy) to the lowest energy state for both even and odd N. We also studied the bulk excitations due to holes. We found some peculiar results for these excitations of this model. Firstly, the number of holes for excited states seem to be reversed: even number of holes for chains with odd number of spins and vice versa. However, one could explain this by resorting to heuristic arguments involving effects of magnetic fields on the spins at the boundary. We then computed the energy due to hole-excitations. We further generalized the finite-size correction calculation to include multi-hole excited states, where these holes are situated to the right of the largest sea root. Having found the correction, we proceeded to compute the effective central charge, $c_{\rm eff}$ and the conformal dimensions, Δ for the model. We found the central charge, $c = 1$. The effective central charge is independent of the boundary parameters, as expected for models with Neumann boundary condition. The result for Δ however, turns out to be similar to models with diagonal boundary terms rather than the nondiagonal ones, to which the model studied here belongs to.

As an independent check to our analytical results, we also solved the model numerically for some large values of N. We used this solution to compute $1/N$ correction for these large N values, then extrapolate them to the $N \to \infty$ limit using Vanden Broeck and Schwartz algorithm. Our numerical results strongly support the analytical derivations presented here. Spectral equivalences between diagonal-nondiagonal and diagonal-diagonal, nondiagonal-nondiagonal and diagonal-diagonal [15, 16, 50] open XXZ spin chains have been shown to exist. Hence, one may attempt to explain the diagonal (Dirichlet) behaviour of the model studied here by some such equivalence. However, to our knowledge, such equivalences have been found when the boundary parameters obey certain constraint [6]–[9], which is not the case for the model we considered here, as already remarked in Footnote 1. Hence, the question about the "Dirichlet-like" behaviour remains for now. We hope to be able to resolve this issue soon.

There are many other open questions that one can explore and address further. For example, similar analysis involving boundary excitations can also be carried out. This can be really challenging even for the diagonal (Dirichlet) case [34, 49]. Further, solution for more general XXZ model involving multiple $Q(u)$ functions [12, 13], can also be utilized

JHEP05(2007)069

in similar capacity to explore these effects. Last but not least, excitations due to other objects that we choose to ignore here, such as special roots/holes and so forth can also be explored for these models in order to make the study more complete. We look forward to address some of these issues in near future.

Acknowledgments

I would like to thank R.I. Nepomechie for his invaluable advice, suggestions and comments during the course of completing this work. I also fully appreciate the financial support received from the Department of Physics, University of Miami.

References

[1] M. Gaudin, *Boundary energy of a Bose gas in one dimension*, *Phys. Rev.* **A 4** (1971) 386; *La fonction d'onde de Bethe*, Masson, Paris (1983).

[2] F.C. Alcaraz, M.N. Barber, M.T. Batchelor, R.J. Baxter and G.R.W. Quispel, *Surface exponents of the quantum XXZ, Ashkin-Teller and Potts models*, *J. Phys.* **A 20** (1987) 6397.

[3] C.J. Hamer, G.R.W. Quispel and M.T. Batchelor, *Conformal anomaly and surface energy for Potts and Ashkin-Teller quantum chains*, *J. Phys.* **A 20** (1987) 5677.

[4] E.K. Sklyanin, *Boundary conditions for integrable quantum systems*, *J. Phys.* **A 21** (1988) 2375.

[5] R.I. Nepomechie, *Solving the open XXZ spin chain with nondiagonal boundary terms at roots of unity*, *Nucl. Phys.* **B 622** (2002) 615 [*Addendum ibid.* **B 631** (2002) 519] [hep-th/0110116].

[6] R.I. Nepomechie, *Functional relations and Bethe ansatz for the XXZ chain*, *J. Statist. Phys.* **111** (2003) 1363 [hep-th/0211001];
Bethe ansatz solution of the open XXZ chain with nondiagonal boundary terms, *J. Phys.* **A 37** (2004) 433 [hep-th/0304092].

[7] J. Cao, H.-Q. Lin, K.-J. Shi and Y. Wang, *Exact solutions and elementary excitations in the XXZ spin chain with unparallel boundary fields*, [cond-mat/0212163];
Exact solution of XXZ spin chain with unparallel boundary fields, *Nucl. Phys.* **B 663** (2003) 487.

[8] R.I. Nepomechie and F. Ravanini, *Completeness of the Bethe ansatz solution of the open XXZ chain with nondiagonal boundary terms*, *J. Phys.* **A 36** (2003) 11391 [*Addendum ibid.* **A 37** (2004) 1945] [hep-th/0307095].

[9] W.-L. Yang, R.I. Nepomechie and Y.-Z. Zhang, *Q-operator and T-Q relation from the fusion hierarchy*, *Phys. Lett.* **B 633** (2006) 664 [hep-th/0511134].

[10] R. Murgan and R.I. Nepomechie, *Bethe ansatz derived from the functional relations of the open XXZ chain for new special cases*, *J. Stat. Mech.* (2005) P05007 [*Addendum ibid* (2005) **P11004**] [hep-th/0504124].

[11] R. Murgan and R.I. Nepomechie, *Generalized T-Q relations and the open XXZ chain*, *J. Stat. Mech.* (2005) P08002 [hep-th/0507139].

[12] R. Murgan, R.I. Nepomechie and C. Shi, *Exact solution of the open XXZ chain with general integrable boundary terms at roots of unity*, *J. Stat. Mech.* (2006) P08006 [hep-th/0605223].

[13] R. Murgan, R.I. Nepomechie and C. Shi, *Boundary energy of the general open XXZ chain at roots of unity*, *JHEP* **01** (2007) 038 [hep-th/0611078].

[14] P. Baseilhac and K. Koizumi, *Exact spectrum of the XXZ open spin chain from the q-Onsager algebra representation theory*, hep-th/0703106.

[15] J. de Gier, A. Nichols, P. Pyatov and V. Rittenberg, *Magic in the spectra of the XXZ quantum chain with boundaries at* $\Delta = 0$ *and* $\Delta = -1/2$, *Nucl. Phys.* **B 729** (2005) 387 [hep-th/0505062].

[16] A. Nichols, V. Rittenberg and J. de Gier, *One-boundary Temperley-Lieb algebras in the XXZ and loop models*, *J. Stat. Mech.* (2005) P03003 [cond-mat/0411512].

[17] I. Affleck, *Universal term in the free energy at a critical point and the conformal anomaly*, *Phys. Rev. Lett.* **56** (1986) 746.

[18] H.W.J. Blötte, J.L. Cardy and M.P. Nightingale, *Conformal invariance, the central charge and universal finite size amplitudes at criticality*, *Phys. Rev. Lett.* **56** (1986) 742.

[19] G. von Gehlen, V. Rittenberg and H. Ruegg, *Conformal invariance and finite one-dimensional quantum chains*, *J. Phys.* **A 19** (1986) 107.

[20] J.L. Cardy, *Conformal-invariance and universality in finite-size scaling*, *J. Phys.* **A 17** (1984) L385;
Operator content of two-dimensional conformally invariant theories, *Nucl. Phys.* **B 270** (1986) 186; *Logarithmic corrections to finite-size scaling in strips*, *J. Phys.* **A 19** (1986) L1093.

[21] H.J. de Vega and F. Woynarovich, *Method for calculating finite size corrections in Bethe ansatz systems: Heisenberg chain and six vertex model*, *Nucl. Phys.* **B 251** (1985) 439.

[22] C.J. Hamer, *Finite-size corrections for ground states of the XXZ Heisenberg chain*, *J. Phys.* **A 19** (1986) 3335.

[23] H.J. de Vega, *Finite-size corrections for nested Bethe Ansatz models and conformal invariance*, *J. Phys.* **A 20** (1987) 6023.

[24] F. Woynarovich and H.-P. Eckle, *Finite-size corrections and numerical calculations for long spin-1/2 Heisenberg chains in the critical region*, *J. Phys.* **A 20** (1987) L97.

[25] F. Woynarovich, *Excitation spectrum of the spin 1/2 Heisenberg chain and conformal invariance*, *Phys. Rev. Lett.* **59** (1987) 259 [*Erratum ibid.* **59** (1987) 1264].

[26] V.I. Inozemtsev and B.-D. Dörfel, *Ground-state energy corrections for antiferromagnetic* $s = 1/2$ *chains with short-range interaction*, *J. Phys.* **A 26** (1993) L999.

[27] B.-D. Dörfel and S. Meissner, *Finite-size corrections of an integrable chain with alternating spins*, *J. Phys.* **A 30** (1997) 1831.

[28] C. Ahn and R.I. Nepomechie, *Finite size effects in the XXZ and sine-Gordon models with two boundaries*, *Nucl. Phys.* **B 676** (2004) 637 [hep-th/0309261].

JHEP05(2007)069

[29] A. Klümper and M.T. Batchelor, *An analytic treatment of finite-size corrections in the spin-1 antiferromagnetic XXZ chain*, *J. Phys.* **A 23** (1990) L189;
A. Klümper and P.A. Pearce, *Analytic calculation of scaling dimensions: tricritical hard squares and critical hard hexagons*, *J. Stat. Phys.* **64** (1991) 13;
A. Klümper, M.T. Batchelor and P.A. Pearce, *Central charges of the 6-vertex and 19-vertex models with twisted boundary-conditions*, *J. Phys.* **A 24** (1991) 3111.

[30] C. Destri and H.J. de Vega, *New thermodynamic Bethe ansatz equations without strings*, *Phys. Rev. Lett.* **69** (1992) 2313; *Non-linear integral equation and excited-states scaling functions in the sine-Gordon model*, *Nucl. Phys.* **B 504** (1997) 621 [hep-th/9701107].

[31] G. Feverati, F. Ravanini and G. Takacs, *Nonlinear integral equation and finite volume spectrum of sine-Gordon theory*, *Nucl. Phys.* **B 540** (1999) 543 [hep-th/9805117].

[32] G. Feverati, *Finite volume spectrum of sine-Gordon model and its restrictions*, hep-th/0001172.

[33] A. LeClair, G. Mussardo, H. Saleur and S. Skorik, *Boundary energy and boundary states in integrable quantum field theories*, *Nucl. Phys.* **B 453** (1995) 581 [hep-th/9503227].

[34] C. Ahn, M. Bellacosa and F. Ravanini, *Excited states NLIE for sine-Gordon model in a strip with Dirichlet boundary conditions*, *Phys. Lett.* **B 595** (2004) 537 [hep-th/0312176].

[35] H. Saleur, *Lectures on non perturbative field theory and quantum impurity problems*, cond-mat/9812110.

[36] I. Affleck, M. Oshikawa and H. Saleur, *Quantum brownian motion on a triangular lattice and $c = 2$ boundary conformal field theory*, *Nucl. Phys.* **B 594** (2001) 535 [cond-mat/0009084].

[37] C. Ahn, R.I. Nepomechie and J. Suzuki, *Finite size effects in the spin-1 XXZ and supersymmetric sine-Gordon models with Dirichlet boundary conditions*, *Nucl. Phys.* **B 767** (2007) 250 [hep-th/0611136].

[38] R. Murgan, R.I. Nepomechie and C. Shi, *Boundary energy of the open XXZ chain from new exact solutions*, *Annales Henri Poincaré* **7** (2006) 1429 [hep-th/0512058].

[39] J-M van den Broeck and L.W Schwartz, *One-parameter family of sequence transformations*, *SIAM J. Math. Anal.* **10** (1979) 658.

[40] C.J. Hamer and M.N. Barber, *Finite-lattice extrapolations for Z_3 and Z_5 models*, *J. Phys.* **A 14** (1981) 2009.

[41] M. Henkel and G. Schütz, *Finite-lattice extrapolation algorithms*, *J. Phys.* **A 21** (1988) 2617.

[42] C. Ahn, Z. Bajnok, R.I. Nepomechie, L. Palla and G. Takacs, *NLIE for hole excited states in the sine-Gordon model with two boundaries*, *Nucl. Phys.* **B 714** (2005) 307 [hep-th/0501047].

[43] H.J. de Vega and A. González Ruiz, *Boundary K matrices for the six vertex and the $n(2n-1)$ A_{n-1} vertex models*, *J. Phys.* **A 26** (1993) L519 [hep-th/9211114].

[44] S. Ghoshal and A.B. Zamolodchikov, *Boundary S matrix and boundary state in two-dimensional integrable quantum field theory*, *Int. J. Mod. Phys.* **A 9** (1994) 3841 [*Erratum ibid.* **A 9** (1994) 4353] [hep-th/9306002].

[45] E.T. Whittaker and G.N. Watson, *A Course of Modern Analysis*, Cambridge University Press (1988).

[46] P.M. Morse and H. Feshbach, *Methods of Theoretical Physics*, New York, McGraw-Hill (1953).

[47] R.I. Nepomechie, private communication.

[48] C.N. Yang and C.P. Yang, *One-dimensional chain of anisotropic spin-spin interactions II. Properties of the ground-state energy per lattice site for an infinite system*, *Phys. Rev.* **150** (1966) 327.

[49] S. Skorik and H. Saleur, *Boundary bound states and boundary bootstrap in the sine-Gordon model with Dirichlet boundary conditions*, *J. Phys.* **A 28** (1995) 6605 [`hep-th/9502011`].

[50] Z. Bajnok, *Equivalences between spin models induced by defects*, *J. Stat. Mech.* (2006) P06010 [`hep-th/0601107`].