The open $XXZ$-chain: bosonization, the Bethe ansatz and logarithmic corrections

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Abstract. We calculate the bulk and boundary parts of the free energy for an open spin-1/2 $XXZ$-chain in the critical regime by bosonization. We identify the cut-off independent contributions and determine their amplitudes by comparing with Bethe ansatz calculations at zero temperature $T$. For the bulk part of the free energy we find agreement with Lukyanov’s result (1998 Nucl. Phys. B 522 533). In the boundary part we obtain a cut-off independent term which is linear in $T$ and determines the temperature dependence of the boundary susceptibility in the attractive regime for $T \ll 1$. We further show that at particular anisotropies where contributions from irrelevant operators with different scaling dimensions cross, logarithmic corrections appear. We give explicit formulae for these terms at those anisotropies where they are most important. We verify our results by comparing with extensive numerical calculations based on a numerical solution of the $T = 0$ Bethe ansatz equations, the finite temperature Bethe ansatz equations in the quantum transfer matrix formalism, and the density matrix renormalization group applied to transfer matrices.

Keywords: integrable spin chains (vertex models), quantum integrability (Bethe ansatz), bosonization, spin chains, ladders and planes (theory)
1. Introduction

The spin-1/2 \textit{XXZ}-chain is described by the Hamiltonian

\[ H = J \sum_{j=1}^{N,N-1} \left[ \frac{1}{2} \left( S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + \Delta S_j^z S_{j+1}^z \right]. \tag{1} \]

Here \( J > 0 \) is the coupling constant and \( N \) is the number of sites. The model is critical for anisotropy \(-1 \leq \Delta \leq 1\). If we take \( N \) as the upper boundary in the sum in equation (1) we have periodic boundary conditions (PBC) whereas taking the sum only up to \( N-1 \) corresponds to open boundary conditions (OBC).

The reasons for the popularity of this model are twofold. On the one hand, this model does indeed capture the basic physics in some real physical systems, for example \( \text{Sr}_2\text{CuO}_3 \) [1]. On the other hand, the model is exactly solvable using the Bethe ansatz. Furthermore, in the continuum limit at low energies it is equivalent to a free boson model up to irrelevant operators. The exact solution at zero temperature \( T \) for the isotropic antiferromagnetic case \( \Delta = 1 \) and PBC was first constructed by Bethe [2]. This so-called

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Bethe ansatz (BA) was later generalized to allow also for the calculation of ground state properties in the anisotropic case [3, 4]. Thermodynamic properties can also be studied by using either the thermodynamic Bethe ansatz (TBA) [5] or the quantum transfer matrix (QTM) approach [6, 7]. However, at finite temperature even the equations obtained for simple thermodynamic quantities like the free energy, specific heat and susceptibility can often only be solved numerically.

The BA solution for the XXZ-chain with OBC at $T = 0$ has been constructed by Gaudin [8], Alcaraz et al [9], and Sklyanin [10]. The application of the TBA for this case seems to be difficult or even impossible as is discussed in more detail in [11, 12]. A modification of the QTM approach is possible as demonstrated in [12] but an evaluation of the formulae obtained still seems to be a formidable task.

An entirely different approach is based on bosonization (see [13] and references therein). Here a low energy effective theory is derived which is just a free boson model up to irrelevant operators. The main advantage of this approach compared to the BA is that any thermodynamic quantity and also any kind of correlation function can be calculated very easily for the free boson model. Corrections to this free boson approximation are obtained by doing perturbation theory in the irrelevant operators. A disadvantage is that the spin-wave velocity $v$, the Luttinger parameter $K$, as well as the amplitudes of the irrelevant terms in the Hamiltonian can only be obtained perturbatively for $|\Delta| \ll 1$. However, one can use the BA to fix $v$ and $K$ which in the language of the bosonic model is equivalent to summing exactly an infinite series of terms which would renormalize the bare values of $v$ and $K$. Lukyanov has demonstrated that the BA can also be used to fix the amplitudes of the leading irrelevant operators in the bosonic model [14]. This allows one to give analytic formulae at low temperatures for the free energy and derived quantities. It also allows one to calculate the correlation amplitudes for the leading and some subleading terms in an asymptotic expansion of spin–spin correlation functions [15].

The XXZ-chain with open boundaries has attracted considerable attention recently [16, 17, 11, 18, 12] because it is the simplest model for a spin chain containing a small number of non-magnetic impurities which cut the chain into parts with essentially free boundaries. It has been shown that the leading irrelevant term in the bosonic model for anisotropy $1/2 < \Delta \leq 1$ leads to a contribution in the boundary susceptibility $\chi_B$ ($O(1)$ part of the susceptibility if the bulk part is $O(N)$) which diverges as $T^{2K-3}$ where the Luttinger parameter $K$ varies between $K = 3/2$ at $\Delta = 1/2$ and $K = 1$ at $\Delta = 1$. The $1/T$ behaviour (up to a logarithmic correction) at the isotropic point is of special interest because it is a Curie-like contribution without any free spins being present. The isotropic ferromagnetic point has also been studied recently [18] and it has been found that the boundary susceptibility $\chi_B \sim -1/T^3$, i.e., the boundary susceptibility diverges more rapidly than and with opposite sign to the bulk susceptibility $\chi \sim 1/T^2$.

In this paper we want to use Lukyanov’s method [14] to obtain explicit expressions for the free energy of the open XXZ-chain for the critical regime $-1 < \Delta < 1$. To do so we will apply perturbation theory in the leading irrelevant operators of the bosonic theory and compare with results obtained using the Bethe ansatz. This will allow us to fix the amplitudes of the irrelevant terms. Our result for the bulk part of the free energy will confirm Lukyanov’s result; however, we will obtain in addition the boundary part. In particular, we find that the boundary susceptibility in the attractive regime behaves as $\chi_B \sim \text{constant} + T$, in contrast to the $\chi_B \sim \text{constant} + T^{2K-3}$ behaviour.

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found before for $0 < \Delta < 1$ [16,17,11]. Another focus of our work is the logarithmic corrections. We will find that the amplitudes in the low temperature expansion of the free energy as well as the amplitudes in the expansion of the ground state energy in terms of the magnetic field $h$ show divergences at infinitely many anisotropies. We will show that these divergences occur because contributions from terms with different scaling dimensions cross at these points. The divergences in the two terms which cross cancel each other, leading to a logarithmic correction. We will give explicit formulae for these corrections at those anisotropies where they are most important.

Our paper is organized as follows. In section 2 we bosonize the open $XXZ$-chain and expand the free energy in powers of $h$, $T$ by using perturbation theory in the leading irrelevant operators. In section 3 we present the zero-temperature Bethe ansatz solution for this model. In particular, we show how the Wiener–Hopf method can be used to obtain leading and next-leading terms in an expansion of the ground state energy in powers of $h$. We then determine the amplitudes of the irrelevant operators in the field theory approach in section 4 by comparing with the BA. We confirm Lukyanov’s result obtained by the same approach for the periodic case. In section 5 we summarize our result for the bulk and boundary part of the susceptibility. We analyse where the amplitudes of the different terms diverge and give explicit formulae for the logarithmic corrections caused, at points where they appear in the leading or subleading term. We check all our analytical results by comparing with a number of numerical data obtained by a numerical solution of the $T = 0$ BA equations, the BA equations in the QTM approach, and the density matrix renormalization group (DMRG) applied to transfer matrices in section 6. In the final section we give a short summary and conclusions.

2. Bosonization for the open chain

First, we want to briefly review the bosonization procedure for the $XXZ$-chain (see for example [13]) to clarify our notation and to remind the reader of how \textit{a priori} unknown parameters in the bosonic model can be determined using the Bethe ansatz.

Using the Jordan–Wigner transformation we can represent the $XXZ$-chain with OBC as given in equation (1) in terms of fermionic operators $\psi_j$:

$$
H = H_0 + H_{\text{int}}
= J \sum_{j=0}^{N} \left[ \frac{1}{2} \left( \psi_j^{\dagger} \psi_{j+1} + \psi_{j+1}^{\dagger} \psi_j \right) + \Delta \left( \psi_j^{\dagger} \psi_j - \frac{1}{2} \right) \left( \psi_{j+1}^{\dagger} \psi_{j+1} - \frac{1}{2} \right) \right]
$$

(2)

where we have added two sites and impose the boundary conditions $\psi_0 = \psi_{N+1} = 0$. For $\Delta = 0$ we are left with a free fermion Hamiltonian $H_0$. The low temperature properties of this model can be studied by linearizing the dispersion around the Fermi points $\pm k_F$ and going to the continuum limit. To do so, we introduce right-and left-moving fermions via

$$
\frac{\psi_j}{\sqrt{a}} \approx e^{ik_F x} \psi_R(x) + e^{-ik_F x} \psi_L(x)
$$

(3)

with $x = ja$, $a$ being the lattice constant. In the half-filled case we have $k_F = \pi/2a$ (no magnetic field applied in (1)). The continuum limit is achieved by using the approximation
The open $XXZ$-chain

\[ \psi_{j+1} = \psi(x) + a \partial_x \psi(x). \]

This leads in lowest order in $a$ to the continuum Hamiltonian

\[ H_0 = iv_0 \int_0^L dx \left[ \psi_R^\dagger \partial_x \psi_R - \psi_L^\dagger \partial_x \psi_L \right] \tag{4} \]

where $L = Na$ and the spin-wave velocity is given by $v_0 = Ja$.

This Hamiltonian can be bosonized by

\[ \psi_R = \frac{1}{\sqrt{2\pi}} \exp(i\sqrt{4\pi} \phi_R); \quad \psi_L = \frac{1}{\sqrt{2\pi}} \exp(-i\sqrt{4\pi} \phi_L) \tag{5} \]

where $\phi = \phi_R + \phi_L$ is a bosonic field obeying the standard commutation rule $[\phi(x), \Pi(x')] = i\delta(x-x')$ with $\Pi = v_0^{-1} \partial_t \phi$. Up to total derivatives the Hamiltonian (4) takes the following form in terms of the bosonic fields:

\[ H_0 = v_0 \int_0^L dx \left[ (\partial_x \phi_R)^2 + (\partial_x \phi_L)^2 \right] = \frac{v_0}{2} \int_0^L dx \left[ \Pi^2 + (\partial_x \phi)^2 \right]. \tag{6} \]

The interaction part of the Hamiltonian (3) can also be expressed in terms of the bosonic fields

\[ H_{\text{int}} = J \Delta \sum_j \left( :\psi_j^\dagger \psi_j : + :\psi_{j+1}^\dagger \psi_{j+1} : \right) \]

\[ \approx \frac{2\Delta v_0}{\pi} \int dx \left[ (\partial_x \phi_R)^2 + (\partial_x \phi_L)^2 + 2(\partial_x \phi_R)(\partial_x \phi_L) \right]. \tag{7} \]

The first two terms are identical to the free part (6) and yield only a renormalization of the velocity

\[ v_0 \rightarrow v = v_0(1 + 2\Delta/\pi). \tag{8} \]

The third term is an interaction between right and left fields. Crucially, even with this term included we still obtain a free boson model in terms of the fields $\phi, \Pi$:

\[ H = H_0 + H_{\text{int}} = \frac{v}{2} \int dx \left[ (1-c)\Pi^2 + (1+c)(\partial_x \phi)^2 \right] \tag{9} \]

with $c = 2\Delta/(\pi + 2\Delta)$. We now rescale the fields via

\[ \phi \rightarrow \frac{\phi}{\sqrt{4\pi} R}; \quad \Pi \rightarrow \sqrt{4\pi} R \Pi; \quad R^2 = \frac{1}{4\pi} \sqrt{\frac{1+c}{1-c}} = \frac{1}{4\pi} \sqrt{1 + \frac{4\Delta}{\pi}} \tag{10} \]

and define the Luttinger parameter

\[ K = \frac{1}{2\pi R^2} = 2 \left( 1 + \frac{4\Delta}{\pi} \right)^{-1/2} \approx 2 - \frac{4\Delta}{\pi}. \tag{11} \]

The bosonized version of the Hamiltonian (1) is then given by

\[ H = \frac{v}{2} \int_0^L dx \left[ \Pi^2 + (\partial_x \phi)^2 \right]. \tag{12} \]

How seriously should one take the values for $v, K$ given in (8) and (11), respectively? We have derived an effective bosonic Hamiltonian for the spin chain by expanding all terms up to linear order in the lattice constant $a$. So clearly, there are higher order corrections.
to the Hamiltonian (12). In fact, there are infinitely many irrelevant terms which have to
be added to this bosonic Hamiltonian to obtain an accurate description of the spin chain.
Some of these terms (in fact, also infinitely many) will further renormalize the values of 
v, K. So equations (8), (11) are perturbative results for v, K expected to be valid only
if |∆| ≪ 1. On the other hand, the model is exactly solvable using the BA and we will
discuss this solution in section 3. Among other things, the BA allows one to calculate
the spin-wave velocity exactly. In other words, the BA allows one to sum up exactly the
infinite perturbative series for v obtained by bosonization. In section 3 we will also see
that the leading term in the bulk susceptibility at zero temperature is a function of v and
K only. This allows it to determine also K exactly and leads to the well known results
\[ v = \frac{\pi \sqrt{1 - \Delta^2}}{2 \arccos \Delta} \] (13)
\[ K = \frac{1}{2\pi R^2} = \frac{\pi}{\pi - \arccos \Delta}. \] (14)

Note that these exact formulae agree with (8), (11) in lowest order in ∆ as expected.
When we use the bosonized Hamiltonian with these values for v, K we should keep in
mind that all contributions from perturbation theory in the irrelevant operators leading
to a renormalization of these parameters are already accounted for.

Finally, we want to give the direct relations between the bosonic and the spin
operators [13] for later use:
\[ S^z_j \approx \frac{1}{2\pi R} \partial_x \phi + (-1)^j \text{ constant } \cos \frac{\phi}{R} \]
\[ S^-_j \approx \exp(2\pi i R \tilde{\phi}) \left( \text{constant } \cos \frac{\phi}{R} + (-1)^j \text{ constant} \right). \] (15)
Here \( \tilde{\phi} = \phi_L - \phi_R \) is the dual field and we clearly have to make the identifications
\( \phi = \phi + 2\pi R \) and \( \tilde{\phi} = \tilde{\phi} + 1/R \), i.e., \( \phi, \tilde{\phi} \) are compact fields.

2.1. The spin chain in a magnetic field and the mode expansion for OBC
When we add a magnetic field term \( H_M = h \sum_{j=1}^{N} S^z_j \) to the Hamiltonian (1), the bosonic
Hamiltonian (12) has to be replaced by
\[ H = \frac{v}{2} \int_0^L dx \left[ \Pi^2 + (\partial_x \phi)^2 - \frac{h}{\pi R v} \partial_x \phi \right] \] (16)
according to equation (15). By performing a shift in the boson field
\[ \phi \rightarrow \phi + hx/(2\pi R v) \] (17)
we can rewrite this as
\[ H = \frac{v}{2} \int_0^L dx \left[ \Pi^2 + (\partial_x \phi)^2 \right] - L \frac{K h^2}{4\pi v}. \] (18)
The bulk susceptibility in lowest order is therefore given by \( \chi_{\text{bulk}} = K/2\pi v \). The magnetic
field shifts the Fermi points away from \( k_F = \pi/2 \) so that according to equation (3) the
right- and left-moving fermions are no longer situated near these points. It is, however,
easy to see that the shift in the Bose field (17) exactly compensates for this shift so that the fermion fields $\psi_R, \psi_L$ belonging to the shifted Bose field have again $k_F = \pi/2$. The boundary conditions for the field $\phi$ in (18) are therefore exactly the same as in a system without a magnetic field.

We first consider the boundary conditions for the $\psi$-field:

$$\psi(0) = \psi(N + 1) = 0$$

$$\Rightarrow \psi_L(0) + \psi_R(0) = 0$$

$$\Rightarrow \psi_L(L) + (-1)^N \psi_R(L) = 0$$  \hspace{1cm} (19)

where $L = Na$ and the last two relations have been derived from (3). From the bosonization formula (5) and the rescaling relation (10) it follows that $[\phi_R(x), \phi_L(x)] = i\pi R^2$ at any site $x \neq 0, L$, i.e., the left and right fields do not commute in general. This is, however, different at the boundaries where $\phi_R, \phi_L$ are related according to (19) leading to $[\phi_R(0), \phi_L(0)] = [\phi_R(L), \phi_L(L)] = 0$ and

$$\phi_R(0) + \phi_L(0) = \pi R + 2\pi R n, \quad \phi_R(L) + \phi_L(L) = 2\pi R n'$$ \hspace{1cm} (20)

where $n$ is an integer. $n'$ is a half-integer if $N$ is even and an integer if $N$ is odd. Equation (15) allows us to fix the numbers $n, n'$ because $S_z^{\text{tot}} = \sum_j S^z_j \approx \frac{[\phi(L) - \phi(0)]}{2\pi R}$.

The total spin $S_z^{\text{tot}}$ should be an integer for $L$ even and a half-integer for $L$ odd. Fixing the boundary condition for $\phi(0)$ we therefore obtain

$$\phi(0) = \pi R; \quad \phi(L) = \pi R + 2\pi R S_z^{\text{tot}}.$$ \hspace{1cm} (21)

This leads to the following mode expansion for OBC [19]:

$$\phi(x, t) = \pi R + 2\pi R S_z^{\text{tot}} \frac{x}{L} + \sum_{n=1}^{N} \frac{\sin(\pi n x/L)}{\sqrt{\pi n}} \left( e^{-i\pi n(\nu t/L)} a_n + e^{i\pi n(\nu t/L)} a_n^\dagger \right),$$ \hspace{1cm} (22)

where $a_n$ is a bosonic annihilation operator.

### 2.2. Correlation functions for the free boson model

From the mode expansion (22) we can directly calculate the basic correlation functions. As we are not interested in finite size effects but rather in the bulk and boundary properties of the chain in the thermodynamic limit, we will consider $L \to \infty$. The results are then valid for the semi-infinite line, i.e., a system with only one boundary.

We start with the basic correlation function

$$\langle \phi(x_1, \tau_1) \phi(x_2, \tau_2) \rangle_{\text{OBC}} \xrightarrow{L \to \infty} -\frac{1}{4\pi} \left( \ln[(x_1 - x_2)^2 + v^2(\tau_1 - \tau_2)^2] - \ln[(x_1 + x_2)^2 + v^2(\tau_1 - \tau_2)^2] \right)$$

$$= \frac{1}{4\pi} \left( \ln(\bar{z}_1 - \bar{z}_2) + \ln(z_1 - \bar{z}_2) - \ln(z_1 - \bar{z}_2) - \ln(\bar{z}_1 - \bar{z}_2) \right)$$ \hspace{1cm} (23)

where $\tau$ represents the imaginary time. In the last line we have introduced new coordinates

$$z = -i(x - \nu t) = v\tau - ix, \quad \bar{z} = i(x + \nu t) = v\tau + ix.$$

\hspace{1cm} (24)
For PBC we would find instead

\[
\langle \phi(x_1, \tau_1)\phi(x_2, \tau_2) \rangle_{\text{PBC}} = \lim_{L \to \infty} \left( -\frac{1}{4\pi} \ln[(x_1 - x_2)^2 + v^2(\tau_1 - \tau_2)^2] + \text{constant} \right) = -\frac{1}{4\pi} \left( \ln(z_1 - z_1) + \ln(\bar{z}_1 - \bar{z}_2) \right) + \text{constant.}
\]

From these basic correlation functions one can easily obtain other correlation functions, for example \( \langle \partial_x \phi \partial_x \phi \rangle \), by taking partial derivatives. The correlation function for the exponential fields can be obtained from

\[
\exp \left( \pm \frac{2\phi(x, \tau)}{R} \right) = \sum_{n=0}^{\infty} \frac{\langle (\pm \frac{2\phi}{R})^n \rangle}{n!} = \sum_{n=0}^{\infty} \frac{(-4/R^2)^n}{(2n)!} \langle \phi^{2n} \rangle
\]

and

\[
\exp \left( \frac{2\phi(x_1, \tau_1)}{R} \right) \exp \left( \pm \frac{2\phi(x_2, \tau_2)}{R} \right) = \exp \left( -\frac{2}{R^2} \langle \phi(x_1, \tau_1) \pm \phi(x_2, \tau_2) \rangle \right)
\]

These formulae for the correlation functions will allow us to calculate the free energy of the model on a semi-infinite line perturbatively in section 2.4.

### 2.3. The free fermion and the free boson model

The free part \( H_0 \) of the Hamiltonian in equation (2) can easily be solved by Fourier transformation. The free energy is given by

\[
F = -T \sum_{n=1}^{N} \ln \left( 1 + e^{-\beta \cos k_n} \right) \quad \text{with} \quad k_n = \frac{\pi}{(N+1)n}
\]

where we set the lattice constant \( a \) and the coupling \( J \) equal to one. The bulk and boundary parts can be obtained by using the Euler–Maclaurin summation formula

\[
F = -\frac{T}{\pi} (N + 1) \int_0^\pi \text{dk} \ln \left( 1 + e^{-\beta \cos k} \right) + \frac{T}{2} \left( \ln(1 + e^\beta) + \ln(1 + e^{-\beta}) \right)
\]

leading to the following low temperature expansion:

\[
F = N \left( -\frac{1}{\pi} - \frac{\pi}{6} T^2 - \frac{7\pi^3}{360} T^4 + O(T^6) \right) + \frac{1}{2} - \frac{1}{\pi} - \frac{7\pi^3}{360} T^2 - \frac{7\pi^3}{360} T^4 + O(T^6) + O(Te^{-1/T}).
\]

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This means that bulk and boundary parts have exactly the same temperature dependence if \( T \ll 1 \). The same is also true for the bulk and boundary susceptibilities \([11]\):

\[
\chi_{\text{bulk}}(h = 0) = \chi_B(h = 0) = \frac{1}{\pi} + \frac{\pi}{6} T^2 + O(T^4).
\]  

(31)

Consider on the other hand the free boson model \([12]\). Using the mode expansion \((22)\) the Hamiltonian takes the form

\[
H = v \sum_{l=1}^{N} \frac{\pi l}{L} \left( a_l^\dagger a_l + \frac{1}{2} \right).
\]  

(32)

To identify the terms which are independent of the details of the dispersion relation we introduce a momentum cut-off \( \Lambda \). The free energy is then given by

\[
F = \sum_{l=1}^{\Lambda N} \frac{v \pi l}{2L} + T \sum_{l=1}^{\Lambda N} \ln \left[ 1 - \exp \left( -\frac{v \pi l}{T L} \right) \right].
\]  

(33)

The first part is the ground state energy \( E_0 \) which is clearly cut-off dependent. We can rewrite the second part and obtain

\[
F = E_0 - T \sum_{n=1}^{\infty} \frac{1}{n} \frac{1 - \exp \left( -\frac{v \pi \Lambda n}{aT} \right)}{\exp \left( \frac{v \pi n}{T L} \right) - 1}.
\]  

(34)

The exponential factor in the numerator is \( \sim O(\exp(-\Lambda/T)) \) and can therefore be ignored if \( T \ll 1 \). If we now consider the limit \( N \to \infty \) with \( T \) fixed we obtain

\[
F = E_0 - L\frac{T^2}{v \pi} \sum_{n=1}^{\infty} \frac{1}{n^2} = E_0 - L\frac{\pi T^2}{6v}.
\]  

(35)

This means that the free energy of the continuum free boson model does not contain any boundary terms. The reason for this is the continuum limit which leads to \( a(N+1) \to Na = L \). All boundary contributions in the field theory therefore have to come from higher order corrections to the free boson model. We expect the same powers of \( T, h \) as are present in the boundary free energy and the boundary susceptibility for the free fermion model (which we will call regular terms subsequently) to also be present for the general case \(-1 < \Delta < 1\) and only the coefficients of these terms to change with anisotropy. By dimensional analysis it becomes clear that the regular terms in boundary quantities obtained by perturbation theory in the irrelevant operators have to involve the short distance lattice cut-off. It is therefore impossible to determine the coefficients of these terms within the field theory approach. We will come back to this point in the next section. The only boundary terms which can be reliably obtained from the field theory are therefore those which have no analogue in the bulk part. Such terms must have an amplitude which vanishes at the free fermion point where bulk and boundary parts show the same dependence on \( T, h \) at low energies.
2.4. Perturbation theory in the irrelevant operators

As we have already mentioned when deriving the bosonic Hamiltonian (12) from the original spin model (1), there are higher order corrections. These corrections are all irrelevant throughout the whole critical regime except for the umklapp term which becomes marginal at \( \Delta = 1 \). This allows it to calculate their effects systematically using simple perturbation theory.

The bosonized Hamiltonian for the spin chain including the irrelevant terms with largest scaling dimensions is given by

\[
H = \frac{v}{2} \int dx \left[ \Pi^2 + (\partial_x \phi)^2 - \frac{h}{\pi Rv} \partial_x \phi \right] + \lambda_1 \int dx \cos \left( \frac{2\phi}{R} \right) \\
+ \frac{\alpha}{\pi^2} \int dx \left[ (\partial_x \phi_R)^2 (\partial_x \phi_L)^2 + a(K)(\partial_x^2 \phi_R)(\partial_x^2 \phi_L) \right] \\
+ \frac{\beta}{\pi^2} \int dx \left[ (\partial_x \phi_R)^4 + (\partial_x \phi_L)^4 + b(K)(\partial_x^2 \phi_R)^2 + (\partial_x^2 \phi_L)^2 \right] 
\]

with \textit{a priori} unknown amplitudes \( \lambda_1, \alpha, \beta \). Here we have separated the terms with integer scaling dimensions into a part where right and left fields are mixed and a part where they remain separated. This will allow us to determine the amplitudes in section 4 by using the fact that no right and left mixing occurs at the free fermion point. The coefficients \( a(K), b(K) \) depend on the Luttinger parameter \( K \) and describe the relative weights of those terms in each bracket with different symmetries. When we shift the \( \phi \)-field again as in (17) the magnetic field appears in the irrelevant terms.

We start with the umklapp term. First-order perturbation theory in \( \lambda_1 \) leads to the correction

\[
F_1^{(1)} = \lambda_1 T \int_0^\beta \int_0^\infty d^2 x \left\langle \cos \left( \frac{2\phi}{R} + \frac{2K h x}{v} \right) \right\rangle_0, 
\]

where \( \langle \cdots \rangle_0 \) means the correlation function calculated for the free boson model. This is the term which has already been considered in [16] and [17] for calculating the leading contribution to the boundary susceptibility and specific heat for \( 1/2 < \Delta < 1 \) at zero magnetic field. We will derive here the more general expression for the free energy contribution at finite temperature and finite magnetic field. Using (26) we obtain at zero temperature

\[
E_1^{(1)} = \lambda_1 \int_0^\infty dx \cos \left( \frac{2K h x}{v} \right) \left( \frac{2}{(2x)^{2K}} \right). 
\]

To obtain the result at small finite temperatures we can use the standard conformal mapping of the complex plane onto a cylinder to replace the correlation function (26) by its finite temperature counterpart so that (38) becomes

\[
F_1^{(1)} = \lambda_1 \int_0^\infty dx \frac{\cos \left( \frac{2K h x}{v} \right)}{\left[ \frac{v}{\pi T} \sinh \left( \frac{2\pi x}{v} \right) \right]^{2K}}. 
\]

The integral is only convergent if \( 0 < 2K < 1 \). On the lattice, convergence will be ensured by a lattice cut-off \( \sim a \) as the lower bound of integration. We can then make the substitution \( x = v \arcsinh(u)/(2\pi T) \) and use partial integration to separate the cut-off
dependent and independent parts. The cut-off independent part is expected to be the same for all $K$ and given by

$$F_1^{(1,\text{conv})} = \frac{\lambda_1 \pi \Gamma(1 - 2K) \left[ \csc(\pi K - i\frac{K h}{2\pi}) + \csc(\pi K + i\frac{K h}{2\pi}) \right]}{4 \Gamma(1 - K - i\frac{K h}{2\pi}) \Gamma(1 - K + i\frac{K h}{2\pi})} \left( \frac{2\pi T}{v} \right)^{2K-1}. \quad (40)$$

There is no bulk contribution in this order of perturbation theory. Taking derivatives with respect to $h$ and $T$, respectively, the known results for the boundary susceptibility and specific heat are obtained [16,17].

To obtain a correction to the bulk free energy we have to go to second order in $\lambda_1$. As the bulk part is not influenced by the boundary conditions and we have already obtained the leading correction to the boundary part in first order we will use PBC to calculate this correction. In this case we have translational invariance leading to

$$f_1^{(2)} = -\frac{\lambda_1^2}{2} \int d^2 x \left\langle \cos \left( \frac{2\phi(x, \tau)}{R} + \frac{2K hx}{v} \right) \right\rangle 0 = -\frac{\lambda_1^2}{4} \int d^2 x \cos \left( \frac{2K hx}{v} \right) \left\langle e^{2i\phi(x, \tau)/R} e^{-2i\phi(0,0)/R} \right\rangle 0. \quad (41)$$

We first consider the case $T = 0$ where this correlation function can be obtained from (25) and (27). The imaginary time integral is given by

$$\int_0^\infty \frac{d\tau}{(x^2 + v^2 \tau^2)^2} = \frac{K \sqrt{\pi} \Gamma(2K - 1/2)}{v \Gamma(2K + 1)} \frac{1}{x^{4K-1}}. \quad (42)$$

This integral is always convergent because we assume $x \geq c$ where $c$ is a lattice cut-off of order $a$. The cut-off independent part of (41) is then given by

$$e_1^{(2,\text{conv})} = \frac{\lambda_1^2}{2} \frac{K \sqrt{\pi} \Gamma(2K - 1/2)}{v \Gamma(2K + 1)} \Gamma(2 - 4K) \cos(2K\pi) \left( \frac{2hK}{v} \right)^{4K-2}. \quad (43)$$

For finite temperatures we can use again the conformal mapping of the plane onto a cylinder for the correlation function. The free energy then becomes

$$f_1^{(2)} = -\frac{\lambda_1^2}{4} \left( \frac{\pi T}{v} \right)^{4K} \int_0^\infty \int_0^\beta \frac{\cos \frac{2K hx}{v} dx d\tau}{[\sinh \frac{x^2}{v}(x + iv\tau) \sinh \frac{x^2}{v}(x - iv\tau)]^{2K}}. \quad (44)$$

To evaluate this integral it is convenient to use the imaginary part of the retarded instead of the imaginary time correlation function and to introduce new variables $u_1 = x - vt$, $u_2 = -x - vt$ leading to

$$f_1^{(2)} = -\frac{\lambda_1^2}{4v} \left( \frac{\pi T}{v} \right)^{4K} \sin(2\pi K) \times \left[ \int_0^\infty \frac{\exp(iKh u/v)}{\sinh^{2K} \frac{x^2}{v} u} du \right] \left[ \int_0^\infty \frac{\exp(-iKh u/v)}{\sinh^{2K} \frac{x^2}{v} u} du \right]. \quad (45)$$

This type of integral can be found to be given by [20]

$$\int_0^\infty du \frac{\exp(iu \zeta)}{\sinh^{2K} \frac{x^2}{v} u} = \frac{2^{2K-1}v}{\pi T} B \left( K - i\frac{v \zeta}{2\pi T}, 1 - 2K \right). \quad (46)$$

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where $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x + y)$. This allows us to obtain the final result

$$f_1^{(2)} = -\frac{\lambda_2^2}{4v} \left(\frac{2\pi T}{v}\right)^{4K-2} \sin(2\pi K) \Gamma^2(1 - 2K)$$

$$\times \frac{\Gamma(K - i\frac{Kh}{2\pi T}) \Gamma(K + i\frac{Kh}{2\pi T})}{\Gamma(1 - K - i\frac{Kh}{2\pi T}) \Gamma(1 + K + i\frac{Kh}{2\pi T})}.$$  \hspace{1cm} (47)

The other irrelevant terms in (36) with amplitudes $\alpha, \beta$ can be expressed as

$$(\partial_x \phi_R)^4 + (\partial_x \phi_L)^4 = \frac{1}{16} \left[ 2(\partial_x \phi)^4 - \frac{12}{v^2}(\partial_x \phi)^2(\partial_x \phi)^2 + \frac{2}{v^4}(\partial_x \phi)^4 \right]$$

$$(\partial_x \phi_R)^2(\partial_x \phi_L)^2 = \frac{1}{16} \left[ (\partial_x \phi)^4 + \frac{2}{v^2}(\partial_x \phi)^2(\partial_x \phi)^2 + \frac{1}{v^4}(\partial_x \phi)^4 \right].$$  \hspace{1cm} (48)

When we now shift the boson field according to (17), terms with an odd number of $\phi$-fields appear. Such terms do not contribute when calculating their expectation value in first-order perturbation theory, because the free boson Hamiltonian consists of an even number of $\phi$-fields. The operators $(\partial_x \phi)^4, (\partial_x \phi)^2(\partial_x \phi)^2, (\partial_x \phi)^4$ and $(\partial_x \phi_R)^2, (\partial_x \phi_L)^2, (\partial_x \phi_R)(\partial_x \phi_L)$ independent of $h$ will only yield a $T^4$-contribution to the bulk part of the free energy [14] and a $T^3$-contribution to the boundary part. The $T^3$-term in the bulk free energy is subleading compared to the $T^4$-term in (35) and we will ignore it. The same is true for the $T^3$-term in the boundary free energy which will be subleading compared to a $T^2$-term which cannot be determined within the field theory approach as discussed at the end of section 2.3.

We therefore have to consider only the following three terms:

$$\frac{AK^2h^4}{4\pi^2v^4}, \quad \frac{3AKh^2}{\pi v^2}(\partial_x \phi)^2, \quad \frac{CKh^2}{2\pi v^2}(\partial_x \phi)^2$$

where we have defined

$$A = \frac{\alpha + 2\beta}{16\pi^2}, \quad C = \frac{2\alpha - 12\beta}{16\pi^2v^2}.$$  \hspace{1cm} (50)

The first term in (49) yields a temperature independent contribution given by

$$f_{A,a}^{(1)} = \frac{AK^2}{4\pi^2v^4}h^4.$$  \hspace{1cm} (51)

The next term gives

$$f_{A,b}^{(1)} = \frac{AT}{L} \frac{3Kh^2}{\pi v^2} \int d^2x \left\langle (\partial_x \phi)^2 \right\rangle.$$  \hspace{1cm} (52)

The correlation function $\left\langle (\partial_x \phi)^2 \right\rangle$ at finite temperature can be obtained by taking derivatives of the correlation function in equation (23) and applying the conformal mapping. To evaluate (52) we will do a point splitting by a small parameter $\epsilon$ in the correlation function. This leads to

$$f_{A,b}^{(1)} = -\frac{3KAh^2T}{2v^4L} \int_0^L dx \left( \frac{1}{\sinh^2 \frac{2\sqrt{v}h}{v} \epsilon} + \frac{1}{\sinh^2 \frac{2\sqrt{v}h}{v}(2x + \epsilon)} \right).$$  \hspace{1cm} (53)
Doing the integral and then expanding in $\epsilon$ yields
\[ f_{A,h}^{(1)} = -\frac{3AKh^2}{2\pi^2v^2\epsilon^2} - \frac{3AKh^2}{4\pi^2v^2L\epsilon} + \frac{AKh^2}{2v^4}T^2 + \frac{1}{L} \frac{3AKh^2}{4\pi^2v^3}T + \mathcal{O}(\epsilon). \] (54)

There are two different ways to interpret this result: one might think of $\epsilon$ as a sort of lattice cut-off. Then one would say that the first term yields a correction to the constant in the bulk susceptibility which depends on this cut-off. However, we have already included all such corrections by using the exact value for the Luttinger parameter $K$, so this term has to be ignored. The second term shows that there is also a constant in the boundary susceptibility; however, it is also cut-off dependent. This means that we cannot determine this constant term within the field theory as expected from the more general discussion in section 2.3. The last two terms which are cut-off independent are therefore the only term we can really determine within the field theory approach. Another point of view is that we should use normal ordered operators. In this case we have to subtract the contributions we can really determine within the field theory approach but will also be calculated in the next section using the BA.

The calculation for the third term in (49) is analogous and the result is
\[ f_{C}^{(1)} = \frac{CKh^2}{4\pi^2\epsilon^2} - \frac{CKh^2}{8\pi^2L\epsilon} - \frac{CKh^2T^2}{12v^2} + \frac{1}{L} \frac{CKh^2T}{8\pi v}. \] (55)

With the help of (50) we can summarize our results for the bulk part of the free energy as follows:
\[ f_{\text{bulk}} = \epsilon_0 - \frac{K}{4\pi v}h^2 + (\alpha + 2\beta)K^2k^4 \frac{64\pi^4v^4}{6v} - \frac{\pi T^2}{6v} + (\alpha + 6\beta)K^2k^2 \frac{48\pi^2v^4}{48\pi^2v^4} \]
\[ - \frac{\lambda_4}{4v} \sin(2\pi K) \Gamma(1 - 2K) \Gamma(K - i\frac{K}{2\pi}) \Gamma(K + i\frac{K}{2\pi}) \left( \frac{2\pi T}{v} \right)^{2K - 2} \] (56)

where $\epsilon_0$ is the ground state energy at zero magnetic field which is known from the BA. The boundary terms calculated using perturbation theory are obtained for the model on the semi-infinite line, i.e., with one boundary. We therefore have to multiply these results by 2. The boundary free energy is then given by
\[ F_B = E_0^B - Bh^2 + \frac{K}{8\pi^3v^3} + \mathcal{O}(T^2, T^4, h^2T^2, \ldots) \]
\[ + \frac{\lambda_1}{2} \frac{\Gamma(1 - 2K) \left[ \csc(\pi K - i\frac{K}{2\pi}) + \csc(\pi K + i\frac{K}{2\pi}) \right]}{\Gamma(1 - K - i\frac{K}{2\pi}) \Gamma(1 - K + i\frac{K}{2\pi})} \left( \frac{2\pi T}{v} \right)^{2K - 1} \] (57)

where $E_0^B$ is the boundary ground state energy in zero magnetic field which we will calculate using the BA in the next section. The constant $B$ cannot be obtained within the field theory approach but will also be calculated in the next section using the BA. $\mathcal{O}(T^2, T^4, h^2T^2, \ldots)$ denotes the regular terms which have been argued to be present in the boundary free energy based on the results for the free fermion model (30). These terms remain undetermined here. The amplitudes $\lambda_1, \alpha$ and $\beta$, on the other hand, can be determined by comparing the field theory with the Bethe ansatz result as was first shown by Lukyanov [14] for the periodic chain. We will show in section 4 that the amplitudes obtained by comparing (56) and (57) with BA calculations for the open chain are consistent with Lukyanov’s result.
3. The Bethe ansatz solution

In this section, leading and next-leading terms in a small field expansion of the ground state energy are calculated within the Bethe ansatz solution for the open chain. Using the Wiener–Hopf procedure, we obtain exact expressions for both the bulk and the boundary contributions. Section 3.2.2 contains an erratum to appendix B in [11].

In order to introduce notation and to make this paper self-contained, the Bethe ansatz is briefly reviewed at the beginning, largely following [8]. We proceed to the thermodynamic limit afterwards. Leading and next-leading contributions to the bulk and boundary susceptibility in terms of the magnetic field are calculated subsequently.

3.1. Coordinate Bethe ansatz for the open $XXZ$-chain

The Hamiltonian (1) conserves the total spin in the $z$-direction $S^z = \sum_{j=1}^{N} S^z_j$, so the eigenvalue of $S^z$ is a good quantum number. Let us denote an eigenstate with $S^z = N/2 - M$ by $|M\rangle$. This eigenstate is a superposition of states with $M$-many $\downarrow$-spins, which we denote by

$$|n_1, \ldots, n_M\rangle = S^-_{n_1} \ldots S^-_{n_M} |0\rangle$$

where $|0\rangle$ is the fully polarized state with $M = 0$. Thus

$$|M\rangle = \sum_{\{n\}} a(n_1, \ldots, n_M) |n_1 \ldots n_M\rangle =: \sum_{\{n\}} a\{n\} |\{n\}\rangle.$$

In terms of the coefficients $a\{n\}$, the eigenvalue equation $H|\{n\} \rangle = E|\{n\} \rangle$ reads

$$\frac{J}{2} \sum_{\{n'\}} (a\{n'\} - \Delta a\{n\}) + \frac{J}{4}(N - 1)a\{n\} = E a\{n\}. \quad (58)$$

Consider the simplified case

$$1 < n_1 < \ldots < n_M < N, \quad n_{j+1} - n_j \geq 1.$$  \quad (59)

Then the $\{n'\}$ are given as function of $\{n\}$, with $n'_\alpha = n_\alpha \pm 1$, so

$$a\{n\} = \exp \left[ i \sum_{j=1}^{M} k_j n_j \right] \quad (60)$$

and

$$\sum_{\alpha=1}^{M} a(n_1, \ldots, n_\alpha + 1, \ldots, n_M) + a(n_1, \ldots, n_\alpha - 1, \ldots, n_M) - 2\Delta a(n_1, \ldots, n_\alpha, \ldots, n_M)$$

$$= 2Ja(n_1, \ldots, n_M). \quad (61)$$

Inserting (60) yields

$$E = J \sum_{j=1}^{M} \cos k_j + J \Delta \left( -M + \frac{N - 1}{4} \right). \quad (62)$$

In solving the full eigenvalue problem (58), two complications arise:
(i) Flipped spins may be nearest neighbours. After acting with \( H \) on a configuration with adjacent spins, amplitudes are obtained where the flipped spins are equal. These amplitudes must vanish. We thus first extend (59),

\[ 1 \leq n_1 \cdots \leq n_M \leq N, \quad (63) \]

and then solve the eigenvalue problem by requiring that (61) and therefore (62) still hold. This means that the following terms in (61) must be zero:

\[ a\left(\ldots, n_\alpha + 1, n_\alpha + 1, \ldots\right) - \Delta a\left(\ldots, n_\alpha, n_\alpha + 1, \ldots\right); \]

\[ a\left(\ldots, n_\alpha, n_\alpha, \ldots\right) - \Delta a\left(\ldots, n_\alpha, n_\alpha + 1, \ldots\right) \]

which leads to

\[ a\left(\ldots, n_\alpha + 1, n_\alpha + 1, \ldots\right) + a\left(\ldots, n_\alpha, n_\alpha, \ldots\right) - 2\Delta a\left(\ldots, n_\alpha, n_\alpha + 1, \ldots\right) = 0. \quad (64) \]

(ii) We have to deal with open boundaries. Therefore, we extend the lattice to include the sites 0 and \( N + 1 \), where transitions to these sites are excluded:

\[ a(0, n_2, \ldots) - \Delta a(1, n_2, \ldots) = 0 \quad (65) \]

\[ a(n_1, \ldots, n_{M-1}, N+1) - \Delta a(n_1, \ldots, n_{M-1}, N) = 0. \quad (66) \]

We expect (i) to lead to a scattering phase in the amplitudes but (ii) to yield the ‘quantization condition’ of the \( k_s \).

In order to solve (i), Bethe [2] constructed the ansatz

\[ a(n_1, \ldots, n_M) = \sum_{P \in \pi_M} A(P) \exp \left[ \sum_{\alpha=1}^{M} k_{P\alpha} n_\alpha \right], \quad (67) \]

where the sum carries over all permutations of \( M \) integers. Then (64) reads

\[ \sum_{P} A(P) \left( e^{i(k_{P\alpha} + k_{P(\alpha+1)})} - 2\Delta e^{i(k_{P\alpha})} + 1 \right) e^{i(k_{P1n_1+\cdots+k_{P\alpha}+k_{P(\alpha+1)n_\alpha+\cdots})} = 0, \quad (68) \]

where \( n_\alpha = n_\alpha + 1 \). Since the terms \( A(P) \) and \( A(PP_{\alpha+1}) \) have the same \( \{n\} \) dependence, (68) is fulfilled if

\[ A(P) \left( e^{i(k_{P\alpha} + k_{P(\alpha+1)})} - 2\Delta e^{i(k_{P\alpha})} + 1 \right) + A(PP_{\alpha+1}) \left( e^{i(k_{P(\alpha+1)}+k_{P\alpha})} - 2\Delta e^{i(k_{P\alpha})} + 1 \right) = 0, \]

from which we conclude that

\[ A(PP_{\alpha+1}) = -A(P)e^{-i\theta_{P\alpha,P(\alpha+1)}} \quad (69) \]

with the scattering phase

\[ e^{-i\theta_{P\alpha,P(\alpha+1)}} = \frac{e^{i(k_{P\alpha} + k_{P(\alpha+1)})} - 2\Delta e^{i(k_{P\alpha})} + 1}{e^{i(k_{P(\alpha+1)}+k_{P\alpha})} - 2\Delta e^{i(k_{P\alpha})} + 1}. \quad (70) \]

From (69), one concludes that

\[ A(P) = e^{2\sum_{\alpha<\beta} \theta_{P\alpha,P\beta}}. \quad (71) \]
If the chain was infinitely long, boundary conditions would not matter and one would choose the \( k_s \) arbitrarily real (mod \( 2\pi \)). However, to take the thermodynamic limit properly and to obtain the boundary contribution to the ground state properties, one applies boundary conditions for the finite system. Here, these are open boundary conditions (for periodic boundary conditions, see [8]).

Before continuing, let us parametrize the \( k_\alpha \) and \( \theta_{\alpha,\beta} \) by roots \( \lambda_\alpha \), such that (70) is fulfilled:

\[
e^{ik_\alpha} = \frac{\sinh(\lambda_\alpha + i\gamma/2)}{\sinh(\lambda_\alpha - i\gamma/2)}
\]

(72)

\[
e^{i\theta(\lambda_\alpha, \lambda_\beta)} = \frac{\sinh(\lambda_\alpha - \lambda_\beta + i\gamma)}{\sinh(\lambda_\alpha - \lambda_\beta - i\gamma)}.
\]

(73)

In order to meet the requirement (ii), the ansatz (67) is modified such that

\[
a(n_1, n_2, \ldots, n_M) = \sum_\{\epsilon\} C(\epsilon_1, \ldots, \epsilon_M) \sum_P \exp \left( i \sum_{\alpha<\beta} \theta(\lambda_{\alpha} - \lambda_{\beta}) + i \sum_{\alpha} k_{P_{\alpha}} n_{\alpha} \right)
\]

(74)

with \( k_\alpha = \epsilon_\alpha |k_\alpha| \), \( \lambda_\alpha = \epsilon_\alpha |\lambda_\alpha| \) and we have defined the \( 2^N \) sets \( \{\epsilon\} \), \( \epsilon_j = \pm 1 \). Note that we have made use of (71) in (67). It is important to note that due to the sum over signs, (74) makes sense only for \( k_\alpha \neq 0, \pm \pi \), that is \( \lambda_\alpha \neq 0, \pm i\pi/2 \) for all \( \alpha \).

The modified ansatz (74) does not influence (72), (73). However, it allows one to meet the open boundary conditions (65), (66). Equation (65) yields

\[
\begin{align*}
C(\epsilon_1, \ldots, \epsilon_{P_{1}}, \ldots, \epsilon_M) & \left( \sum_{\alpha \neq 1} e^{i(\epsilon_{P_{1}} - \lambda_{P_{\alpha}}) + \Delta e^{ik_{P_{1}}}} \right) \\
+ C(\epsilon_1, \ldots, -\epsilon_{P_{1}}, \ldots, \epsilon_M) & \left( \sum_{\alpha \neq 1} e^{-i(\epsilon_{P_{1}} + \lambda_{P_{\alpha}}) - \Delta e^{-ik_{P_{1}}}} \right) = 0.
\end{align*}
\]

(75)

From (70),

\[
e^{-i\theta(2\lambda_\alpha)} = \frac{1 - \Delta e^{-ik_\alpha}}{1 - \Delta e^{ik_\alpha}},
\]

(76)

so (75) becomes

\[
\frac{C(\epsilon_1, \ldots, -\epsilon_{P_{1}}, \ldots, \epsilon_M)}{C(\epsilon_1, \ldots, \epsilon_{P_{1}}, \ldots, \epsilon_M)} = \exp \left( i \sum_{\beta \neq \alpha} \theta(\lambda_{\alpha} - \lambda_{\beta}) + \theta(\lambda_{\alpha} + \lambda_{\beta}) + 2\theta(2\lambda_\alpha) \right)
\]

with the unique solution

\[
C(\epsilon_1, \ldots, \epsilon_M) = \exp \left( -i \sum_{\alpha \leq \beta} \theta(\lambda_{\alpha} + \lambda_{\beta}) \right).
\]

We thus have the amplitude

\[
a\{n\} = \sum_P \sum_\{\epsilon\} \exp \left( i \sum_{\alpha<\beta} \theta(\lambda_{\alpha} - \lambda_{\beta}) - \theta(\lambda_{\alpha} + \lambda_{\beta}) \right) - i \sum_{\alpha} \theta(2\lambda_{\alpha}) + i \sum_{\alpha} n_{\alpha} k_{P_{\alpha}} \right).
\]
This expression is substituted into equation (66) to obtain
\[
e^{iNkPM} \left( e^{ikPM} - \Delta \right) \exp \left( \frac{i}{2} \sum_{\alpha \leq M} \theta(\lambda_{\alpha} - \lambda_{PM}) - \theta(\lambda_{\alpha} + \lambda_{PM}) \right)
+ e^{-iNkPM} \left( e^{-ikPM} - \Delta \right) \exp \left( \frac{i}{2} \sum_{\alpha \leq M} \theta(\lambda_{\alpha} + \lambda_{PM}) - \theta(\lambda_{\alpha} - \lambda_{PM}) \right) = 0.
\]

(77)

Note that the ks are parametrized by the \( \lambda \)s via (72). Using (76), equation (77) is written as
\[
\frac{a^{2(N+1)}(\lambda_k, \gamma/2)}{a^{2(N+1)}(\lambda_k, -\gamma/2)} \frac{a(2\lambda_k, -\gamma)}{a(2\lambda_k, \gamma)} = -\frac{q_M(\lambda_k + i\gamma)q_M(-\lambda_k - i\gamma)}{q_M(\lambda_k - i\gamma)q_M(-\lambda_k + i\gamma)},
\]

with the definitions
\[
a(\lambda, \mu) := \sinh(\lambda + i\mu), \quad q_M(\lambda) := \prod_{j=1}^{M} \sinh(\lambda - \lambda_j).
\]

This equation is equivalent to
\[
\left[ \frac{a(\lambda_k, \gamma/2)}{a(\lambda_k, -\gamma/2)} \right]^{2N} \left[ \frac{a(2\lambda_k, \gamma)a(\lambda_k, \pi/2 - \gamma/2)a(\lambda_k, \pi/2 - \gamma/2)}{a(2\lambda_k, -\gamma)a(\lambda_k, -\pi/2 + \gamma/2)a(\lambda_k, -\pi/2 + \gamma/2)} \right] = -\frac{q_M(\lambda_k + i\gamma)q_M(-\lambda_k - i\gamma)}{q_M(\lambda_k - i\gamma)q_M(-\lambda_k + i\gamma)},
\]

which also follows from the algebraic Bethe ansatz [10]. The equations (78) are the above-mentioned ‘quantization conditions’ on the \( \lambda \)s and therefore on the ks.

The energy (62), including a magnetic field \( h \) along the \( S^z \)-direction, reads in terms of the \( \lambda \)s
\[
E = J \left[ -\sum_{j=1}^{M} \frac{\sin^2 \gamma}{\cosh(2\lambda_j) - \cos \gamma} + \frac{N-1}{4} \cos \gamma \right] - hS^z
\]
\[
S^z = N/2 - M.
\]

(80)

(81)

The distribution of the roots has been investigated in [11]. There it has been shown that the equations (79) can be symmetrized by introducing the set of roots \( \{v_1, \ldots, v_N\} := \{-\lambda_{N/2}, \ldots, -\lambda_1, \lambda_1, \ldots, \lambda_{N/2}\} \), whose elements are distributed symmetrically on the real axis w.r.t. the origin. The \( v_j \) are the \( N \) real solutions to the equations
\[
\left[ \frac{a(\lambda_k, \gamma/2)}{a(\lambda_k, -\gamma/2)} \right]^{2N} \left[ \frac{a(v_m, \pi/2 - \gamma/2)a(v_m, \gamma/2)}{a(v_m, -\pi/2 + \gamma/2)a(v_m, -\gamma/2)} \right] = \frac{q_N(v_m + i\gamma)}{q_N(v_m - i\gamma)}.
\]

(82)

Note that \( \pm i\pi/2, 0 \) are solutions of (82). However, these solutions are not permitted within the Bethe ansatz as explained after equation (74).\(^3\) This is a direct consequence of the broken translational symmetry in the open system.

\(^3\) Within the algebraic Bethe ansatz, the creation operators which are used to create eigenvectors by acting on a reference state are identically zero at spectral parameters \( 0, \pm i\pi/2 \). This can be seen directly from Sklyanin’s work [10].
3.2. $T = 0$ properties in the thermodynamic limit

To pass to the thermodynamic limit, it is convenient to define the density of roots on the real axis, $\rho(x)$. In [11], the following linear integral equation has been derived for $\rho(x)$:

$$\vartheta(x, \gamma) + \frac{1}{2N} \left[ \vartheta(x, \gamma) + \vartheta(x, \pi - \gamma) + \vartheta(x, 2\gamma) \right] = \rho(x) + \int_{-B}^{B} \vartheta(x - y, 2\gamma) \rho(y) \, dy, \quad (83)$$

where

$$2\pi i \vartheta(x, \gamma) := \frac{2i \sin \gamma}{\cosh 2x - \cos \gamma} = \frac{d}{dx} \ln \frac{\sinh(x + i\gamma/2)}{\sinh(x - i\gamma/2)} = i \frac{d}{dx} k(x). \quad (84)$$

This equation is valid including the order $O(1/N)$, that is, including the bulk and the boundary contributions.

Equation (83) is a linear integral equation with two unknowns, $B$ and $\rho$. In a first step, (83) is solved for $B = \infty$; in a second step, $\rho(x)$ is obtained depending on the parameter $B$ and the dependence of $B$ on the magnetic field $h$ is calculated. We will see that $B = \infty$ corresponds to $h = 0$, and a finite magnetic field $h > 0$ induces a finite $B < \infty$. Finally, the susceptibility $\chi(h)$ is deduced. This procedure is reviewed in [5].

It will be shown later that instead of dealing with $\rho$, all quantities that we are interested in can be expressed more conveniently by $g_+(x) := \theta(x) \rho(x + B)$. The calculation of these functions is done by Fourier transformation,

$$\rho(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{\rho}(k) e^{-ikx} \, dk. \quad (86)$$

Let us first consider the case $B = \infty$. It is straightforward to solve (83) in Fourier space, where

$$\tilde{\vartheta}(k, \gamma) = \frac{\sinh(\pi/2 - \gamma/2)k}{\sinh \pi k/2}. \quad (85)$$

We denote the solution of (83) for $B = \infty$ by $\rho_0$ and find

$$\tilde{\rho}_0(k) = \tilde{s}(k) + \frac{1}{2N} \frac{\cosh \gamma k/4 \cosh(\pi/4 - \gamma/2)k}{\cosh \gamma k/2 \cosh(\pi - \gamma)k/4}, \quad (87)$$

with

$$\tilde{s}(k) := \frac{1}{2 \cosh \gamma k/2}, \quad s(x) = \frac{1}{2 \gamma \cosh \pi x/\gamma}. \quad (87)$$

Note that $\int_{-\infty}^{\infty} \rho_0(x) \, dx = 1/2 + 1/(2N)$, which corresponds to $M = N/2$ in equation (82). Putting this into equation (81), one has $S^z = 0$. Thus a vanishing magnetic field corresponds to $B = \infty$. This means that in order to perform a small field expansion $|h| \ll \alpha$ (where $\alpha$ is some scale which is determined later), one has to asymptotically expand the energy as $B \to \infty$.

To do so, we now consider the case $B < \infty$, i.e., a finite magnetic field. Using (85) we can rewrite (83) as

$$\rho(x) = \rho_0(x) + \int_{|y| > B} \kappa(x - y) \rho(y) \, dy \quad (86)$$

$$\kappa(x) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\sinh(\pi/2 - \gamma)k}{2 \cosh \gamma k/2 \sinh(\pi - \gamma)k/2} e^{-ikx} \, dk. \quad (87)$$

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The functions
\[ G \quad \tilde{\gamma} \quad \tilde{g} \quad \rho \]

The driving term \( \tilde{\gamma} \) is explained for example in \([21, 22]\).

Thus in each order, a linear integral equation of Wiener–Hopf type has to be solved. This technique is explained for example in \([21, 22]\).

The first two orders of \( \tilde{g}_+(k) \) read
\[ \tilde{g}_+^{(1)}(k) = G_+(k) \left[ \tilde{\rho}_0(k) G_-(-k) e^{-ikB} \right]_+^{(1)} \]
\[ \tilde{g}_+^{(2)}(k) = G_+(k) \left\{ \left[ \tilde{\rho}_0(k) G_-(-k) e^{-ikB} \right]_+^{(2)} + \left[ \tilde{\kappa}(k) \tilde{g}_+^{(1)}(-k) G_-(-k) e^{-2ikB} \right]_+ \right\}, \]

where the indices \( \pm \) are defined by
\[ f_\pm(k) := \pm \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{f(q)}{k - q \pm i\varepsilon} dq. \]

The functions \( G_\pm(k) \) are obtained from the factorization \( 1 - \tilde{\kappa} = 1/(G_+ G_-) \); they read
\[ G_+(k) = \frac{\sqrt{2(\pi - \gamma)}}{\Gamma(1/2 - i\gamma k/(2\pi)) \Gamma(1 - ik/\pi)} e^{-iak} \]
\[ a = \frac{1}{2} \left[ \frac{\gamma}{\pi} \ln(\pi/\gamma - 1) - \ln(1 - \gamma/\pi) \right] \]
\[ G_-(k) = G_+(-k). \]

We restrict ourselves to the calculation of \( \tilde{g}_+ \), which is sufficient for our purposes.

The bracket \( \ldots \) in \( \tilde{g}_+^{(1)} \) and the first term in \( \tilde{g}_+^{(2)} \) are evaluated using \( \gamma \). We thus have to find the residues of
\[ \frac{1}{2 \cosh \frac{x_k}{2}} \quad \frac{\cosh \frac{\pi}{2} \cosh \left( \frac{x_k}{2} - \frac{\pi}{2} k \right) k}{\cosh \frac{\pi}{2} \cosh \frac{\pi}{4} k} \]
at the poles closest to the real axis in the lower half-plane (the first term in the above line accounts for the bulk contribution, the second for the boundary contribution from \([85]\)).

This is done straightforwardly for the bulk part: the poles are located at
\[ k_n^{(1)} = -i(2n + 1)\pi/\gamma, \quad n = 0, 1, \ldots. \]
The relevant poles of the boundary part, however, depend on whether $\gamma < \pi / 3$ or $\gamma > \pi / 3$: poles at $k^{(1)}_m$ are found as well as poles at
\[
k^{(2)}_m = -i2(m+1)\pi / (\pi - \gamma), \quad m = 0, 1, \ldots
\]
(99)
For $\gamma > \pi / 3$, the leading pole is $k^{(1)}_0$, whereas for $\gamma < \pi / 3$, the pole $k^{(2)}_0$ is leading. Finally double poles occur at
\[
\gamma = \frac{2n+1}{4m+2n+3}, \quad k^{(1,2)}_{m,n} = -i(4m+2n+3)\pi / (\pi - \gamma), \quad m,n = 0, 1, \ldots
\]
(100)
where the leading and next-leading ones occur for $\gamma = \pi / 3, 3\pi / 5$. In the following, we will concentrate on the single poles, i.e. $\gamma \neq \pi / 3$ in the leading order and $\gamma \neq \pi / 3, 3\pi / 5$ in the next-leading order. The extension of the results to the cases $\gamma = \pi / 3, 3\pi / 5$ is discussed in section 5. We first consider the leading order contributions (92), before proceeding to the next-leading corrections (93). The isotropic case $\gamma = 0$ is treated separately.

3.2.1. The leading orders. By taking only the poles $k^{(1)}_0$, $k^{(2)}_0$ nearest to the real axis into account, one finds for $\gamma \neq \pi / 3$
\[
\tilde{g}^{(1)}_+ (k) = G_+(k) \left\{ \frac{a_0}{k+i\pi/\gamma} e^{-\pi B/\gamma} + \frac{1}{2N} \left[ \frac{a_1}{k+i\pi/\gamma} e^{-\pi B/\gamma} \right] + \left[ \frac{b_1}{k+i2\pi/ (\pi - \gamma)} e^{-2\pi B/ (\pi - \gamma)} \right] \right\}. 
\]
(101)
We could proceed analogously for $\gamma = \pi / 3$ by evaluating the residue at the double pole [11]. However, it turns out to be more convenient to include the point $\gamma = \pi / 3$ only at the very end, once the susceptibility has been calculated. The constants in (101) are given by
\[
a_0 = \frac{i}{\gamma} G_- (-i\pi/\gamma),
\]
(102a)
\[
a_1 = \frac{\sqrt{2}i}{\gamma} G_- (-i\pi/\gamma) \frac{\sin \pi^2 / (4\gamma)}{\cos \pi^2 / (4\gamma) - \pi / 4},
\]
(102b)
\[
b_1 = \frac{2i}{\pi - \gamma} \tan \pi \gamma / (\pi - \gamma) G_- (-i2\pi/ (\pi - \gamma)).
\]
(102c)
We can now compute $s^z := S^z / N$ and $e := E / N$ from (80), (81):
\[
s^z = 1/2 - \int_{-B}^B \rho(x) \, dx + 1/(2N)
\]
(103)
\[
e = -hs^z - J \frac{\sin \gamma}{2} \int_{-B}^B \vartheta(x, \gamma) \rho(x) \, dx + \frac{J}{4} \left( \cos \gamma + \frac{2 - \cos \gamma}{N} \right).
\]
(104)
We insert (86) into (103) to obtain
\[
s^z = \frac{\pi}{\pi - \gamma} \tilde{g}_+ (0),
\]
(105)
which is an exact statement, including all orders $\tilde{g}^{(n)}$. It is convenient to calculate $e - e_0$, where $e_0 := e (h = 0)$ is the ground state energy at zero magnetic field. From (85), (104)
one finds
\[
e_0 = \frac{J}{4} \left( \cos \gamma + \frac{2 - \cos \gamma}{N} \right) - \frac{J}{2} \sin \gamma \int_{\gamma}^{\infty} \vartheta(x, \gamma) \rho_0(x) \, dx
\]
\[
= \frac{J}{4} \cos \gamma - \frac{J}{4} \sin \gamma \int_{\gamma}^{\infty} \frac{\sinh(\pi/2 - \gamma/2) k}{2 \cosh \gamma k/2 \sinh \pi k/2} \, dk + \frac{1}{N} \left[ \frac{J(2 - \cos \gamma)}{4} \right]
\]
\[
- \frac{J}{4} \sin \gamma \int_{\gamma}^{\infty} \frac{\cosh \gamma k/4 \cosh(\pi/4 - \gamma/2) k}{2 \cosh \gamma k/2 \cosh(\pi - \gamma/2) k} \sinh(\pi/2 - \gamma/2) k \, dk \bigg] . \tag{106}
\]

We use again (86) which yields
\[
e - e_0 = -h s^z + \frac{4J\pi \sin \gamma}{\gamma} \int_{0}^{\infty} \frac{g_+(x)}{\cosh(x + B)\pi/\gamma} \, dx
\]
\[
= -\frac{h\pi}{\pi - \gamma} \left( \tilde{g}^{(1)}_+(0) + \tilde{g}^{(2)}_+(0) \right) + \frac{8\pi J \sin \gamma}{\gamma} \left[ \left( \tilde{g}^{(1)}_+(i\pi/\gamma) + \tilde{g}^{(2)}_+(i\pi/\gamma) \right) e^{-\pi B/\gamma}
\]
\[
- \tilde{g}^{(1)}_+(3i\pi/\gamma) e^{-3\pi B/\gamma} + O(e^{-3\pi B/\gamma}) \bigg] , \tag{107}
\]
where in the last equation we restrict ourselves to the given orders. Now \(B\) is treated as a variational parameter and is determined in such a way that
\[
\frac{\partial}{\partial B}(e - e_0) = 0. \tag{108}
\]

In this section we consider only the leading order in (107). Inserting (101), (105), (107) in (108), \(B\) is obtained as a function of \(h\):
\[
B = -\frac{\gamma}{\pi} \ln \frac{h}{\alpha} \tag{109}
\]
\[
\alpha := \frac{2\pi J \sin \gamma (\pi - \gamma)}{\gamma} \frac{G_+(i\pi/\gamma)}{G_+(0)}. \tag{110}
\]

Thus \(\alpha\) sets the scale for \(h\) (this scale \(\alpha\) should not be confused with the amplitude \(\alpha\) introduced in section 2). The restriction to the leading orders in \(\exp[-B]\) is equivalent to the leading orders in \(h\) in the limit \(|h| \ll \alpha\).

One now makes use of (110) to determine \(s^z(h)\) from (105), and therefrom \(\chi(h) = \partial s^z/\partial h\). Inserting the expressions for \(G_\pm\) from equations (95), (96) we find
\[
\chi_{\text{bulk}} = \frac{\gamma}{(\pi - \gamma) \pi J \sin \gamma}. \tag{111a}
\]

This result is well known; see, for example, [5]. The boundary contribution is given by
\[
\chi_B(h) = \frac{\gamma}{J(\pi - \gamma) \pi \sqrt{2} \sin \gamma} \frac{\sin \pi^2/(4\gamma)}{\cos(\pi^2/(4\gamma) - \pi/4)}
\]
\[
+ \frac{2\gamma \sqrt{\pi}}{(\pi - \gamma)^2} \tan \frac{\pi \gamma}{\pi - \gamma} \frac{1}{\alpha} \frac{\Gamma(\pi/(\pi - \gamma))}{\Gamma((1/2 + \gamma)/(\pi - \gamma))} \Gamma((1 + \pi/(2\gamma))/((\pi - \gamma)) (h/\tilde{\alpha})^{-(\pi - 3\gamma)/(\pi - \gamma)} \tag{111b}
\]
for \(\gamma \neq \pi/3\) with
\[
\tilde{\alpha} = 2J(\pi - \gamma) \sqrt{\pi} \frac{\sin \gamma \Gamma(1 + \pi/(2\gamma))}{\Gamma((1/2 + \pi/(2\gamma))}. \tag{111c}
\]
Note that the first term in (111b), which is independent of the magnetic field $h$, is the leading contribution for $\gamma > \pi/3$ (the pole closest to the real axis in (92)). For $\gamma < \pi/3$ the second term dominates. The question of to what extent the result (111b) also yields the next-leading corrections for the whole range of $0 < \gamma < \pi$ cannot be answered at this point: so far, we have only focused on the leading poles. Next-leading corrections will be discussed in the next section.

The constant contribution in (111b), as well as the pre-factor of the $h$ dependent part, show divergences for certain values of $\gamma$. We will comment on these in section 5.

3.2.2. The next-leading orders. In this section, the Wiener–Hopf result (93) in (107), (105) is used to calculate next-leading corrections to (111b). This section also constitutes an erratum to appendix B in [11].

Let us start with the bulk contribution. We already commented on the calculation of the first term in (93) after that equation. The second term involves the residues of $\tilde{\kappa}(k)$ at the poles closest to the real axis. As can be seen from (87), poles occur at $k_n^{(1)}$ (cf equation (98)) and at

$$k_l^{(3)} = -\frac{i}{\pi - \gamma} \frac{2\pi}{l}, \quad l = 1, 2, \ldots$$

This situation is very similar to the leading order of the boundary contribution.

The boundary contribution is treated analogously. The only difference is that the function $\tilde{g}_+(k)$ given in (101) contains two terms in $1/N$. The first term obviously yields exponents in analogy to the bulk. The second one has poles given in equation (99) which have to be combined with those in equation (112).

In the following, we will focus on the amplitudes of the most important next-leading terms, that is, we consider the residues due to $k_0^{(1)}$ and $k_0^{(3)}$ in the second term in (93). Calculating the residua mentioned above and putting everything together, one ends up with

$$\tilde{g}_+^{(2)}(k) = G_+(k)$$

$$\times \left\{ \left( \frac{a_{0,1}}{k + i3\pi/\gamma} + \frac{a_{0,2}}{k + i\pi/\gamma} \right) e^{-3\pi B/\gamma} + \frac{a_{0,3}}{k + i2\pi/(\pi - \gamma)} e^{-(\pi/\gamma + 4\pi/(\pi - \gamma))B} + \frac{1}{2N} \left[ \left( \frac{a_{1,1}}{k + i3\pi/\gamma} + \frac{a_{1,2}}{k + i\pi/\gamma} \right) e^{-3\pi B/\gamma} + \frac{a_{1,3}}{k + i2\pi/(\pi - \gamma)} e^{-(\pi/\gamma + 4\pi/(\pi - \gamma))B} + \left( \frac{b_{1,1}}{k + i6\pi/(\pi - \gamma)} + \frac{b_{1,3}}{k + i2\pi/(\pi - \gamma)} \right) e^{-6\pi B/(\pi - \gamma)} + \frac{b_{1,2}}{k + i\pi/\gamma} e^{-2(\pi/\gamma + \pi/(\pi - \gamma))B} \right] \right\}$$

$$a_{0,1} = \frac{i}{\gamma} G_- \left( \frac{-3\pi}{\gamma} \right)$$

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\[ a_{0,2} = \frac{i}{2\gamma \pi} \tan \frac{\pi^2}{2\gamma} G^3_-(\frac{-i\pi}{\gamma}) \]  
(115)

\[ a_{0,3} = \frac{i}{\pi(\pi + \gamma)} \tan \frac{\pi\gamma}{\pi - \gamma} G_-\left(\frac{-i\pi}{\gamma}\right) G^2_-\left(\frac{-i2\pi}{\pi - \gamma}\right) \]  
(116)

\[ a_{1,1} = \frac{2 \sin \pi/4 \sin 3\pi^2/(4\gamma)}{\gamma \cos(3\pi^2/(4\gamma) + \pi/4)} G_-\left(\frac{-3\pi}{\gamma}\right) \]  
(117)

\[ a_{1,2} = \frac{a_1}{2\pi} \tan \frac{\pi^2}{2\gamma} G_-\left(\frac{-i\pi}{\gamma}\right) \]  
(118)

\[ a_{1,3} = \frac{a_1 \gamma}{\pi(\pi + \gamma)} \tan \frac{\pi\gamma}{\pi - \gamma} G^2_-\left(\frac{-i2\pi}{\pi - \gamma}\right) \]  
(119)

\[ b_{1,1} = \frac{i}{\pi - \gamma} \tan \frac{3\pi}{\pi - \gamma} G_-\left(\frac{-i6\pi}{\pi - \gamma}\right) \]  
(120)

\[ b_{1,2} = \frac{b_1(\pi - \gamma)}{\pi(\pi + \gamma)} \tan \frac{\pi^2}{2\gamma} G_-\left(\frac{-i\pi}{\gamma}\right) \]  
(121)

\[ b_{1,3} = \frac{b_1}{4\pi} \tan \frac{\pi\gamma}{\pi - \gamma} G_-\left(\frac{-i2\pi}{\pi - \gamma}\right) \]  
(122)

This expression for $\tilde{g}_2$ is inserted into (107), where we now have to keep all the terms indicated. Then $B$ as a function of $h$ is derived. In section 3.2.1, we found that this relationship is the same both for the boundary and for the bulk in the leading order. This is no longer true when next-leading terms are considered. For the bulk we obtain

\[ \alpha e^{-\pi B/\gamma} = h \left( 1 + A_1 \left(\frac{h}{\alpha}\right)^2 + A_2 \left(\frac{h}{\alpha}\right)^{4\gamma/(\pi - \gamma)} \right) \]  
(123)

\[ A_1 = \frac{a_{0,2}}{a_0} + \frac{G_-(-i3\pi/\gamma)}{G_-(-i\pi/\gamma)}, \quad A_2 = \frac{\pi - \gamma}{2\gamma} \frac{a_{0,3}}{a_0}. \]

Care has to be taken in inverting the relation $h = h(B)$ in order to get $B = B(h)$ for the boundary: this is done by performing an expansion for large $B$ in $h = h(B)$. The next-leading terms in this expansion depend on the range of $\gamma$, whether $\gamma < \pi/3$ or $\gamma > \pi/3$. In the final result $B = B(h)$, the parameter $\gamma$ must enter uniquely. Then we find

\[ \alpha e^{-\pi B/\gamma} = h \left( 1 + A_1 \left(\frac{h}{\alpha}\right)^2 + A_2 \left(\frac{h}{\alpha}\right)^{4\gamma/(\pi - \gamma)} \right) \]  
(124)

\[ A_1 = \frac{a_{1,2}}{a_1} + \frac{G_-(-i3\pi/\gamma)}{G_-(-i\pi/\gamma)}, \quad A_2 = \frac{\pi - \gamma}{2\gamma} \frac{a_{1,3}}{a_1}. \]  
(125)

Here terms of higher order, previously given in [11], have been discarded for the reason mentioned above.

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Combining these equations with (105), one finds
\[ s_{\text{bulk}}^2(h) = \sqrt{\frac{2}{\pi(\pi-\gamma)}} \left\{ G_-(-i\pi/\gamma) \frac{1}{\alpha} \right. \\
+ \left( \frac{1}{\pi} \tan \frac{\pi^2}{2\gamma} G_+^3 \left( -i\frac{\pi}{\gamma} \right) + \frac{2}{3} G_- \left( -i\frac{3\pi}{\gamma} \right) \right) \left( \frac{h}{\alpha} \right)^3 \\
+ \frac{\pi-\gamma}{\pi(\pi+\gamma)} \tan \frac{\pi\gamma}{\pi-\gamma} G_- \left( -i\frac{\pi}{\gamma} \right) G_+^2 \left( -i\frac{2\pi}{\pi-\gamma} \right) \left( \frac{h}{\alpha} \right)^{1+4\gamma/(\pi-\gamma)} \right\} \] (126)

\[ s_{\text{B}}^2(h) = -i \sqrt{\frac{1}{2\pi(\pi-\gamma)}} \left\{ \gamma a_1 \frac{h}{\alpha} + \frac{\pi-\gamma}{2} \frac{b_1}{h} \left( \frac{h}{\alpha} \right)^{2\gamma/(\pi-\gamma)} \right. \\
+ \left( 2\gamma a_{1,2} + \frac{\gamma}{3} a_{1,1} + \gamma a_1 G_+ (i3\pi/\gamma) \right) \left( \frac{h}{\alpha} \right)^3 \\
+ \frac{3\gamma + \pi}{\alpha\pi(\pi+\gamma)} \tan \frac{\pi\gamma}{\pi-\gamma} G_- \left( -i\frac{\pi}{\gamma} \right) G_+^2 \left( -i\frac{2\pi}{\pi-\gamma} \right) \left( \frac{h}{\alpha} \right)^{4\gamma/(\pi-\gamma)} \right\} \] (127)

These results correct those of [11]. From these expressions, \( \chi_{\text{bulk}} \) and \( \chi_{\text{B}} \) can be obtained:
\[ \chi_{\text{bulk}}(h) = \sqrt{\frac{2}{\pi(\pi-\gamma)}} \left\{ G_-(-i\pi/\gamma) \frac{1}{\alpha} \right. \\
+ \frac{3}{\alpha} \left( \frac{1}{\pi} \tan \frac{\pi^2}{2\gamma} G_+^3 \left( -i\frac{\pi}{\gamma} \right) + \frac{2}{3} G_- \left( -i\frac{3\pi}{\gamma} \right) \right) \left( \frac{h}{\alpha} \right)^2 \\
+ \frac{3\gamma + \pi}{\alpha\pi(\pi+\gamma)} \tan \frac{\pi\gamma}{\pi-\gamma} G_- \left( -i\frac{\pi}{\gamma} \right) G_+^2 \left( -i\frac{2\pi}{\pi-\gamma} \right) \left( \frac{h}{\alpha} \right)^{4\gamma/(\pi-\gamma)} \right\} \] (128)

\[ \chi_{\text{B}}(h) = -i \sqrt{\frac{1}{2\pi(\pi-\gamma)}} \left\{ \gamma a_1 \frac{h}{\alpha} + \frac{\gamma}{h} \frac{b_1}{\alpha} \left( \frac{h}{\alpha} \right)^{2\gamma/(\pi-\gamma)-1} \right. \\
+ \frac{3}{\alpha} \left( 2\gamma a_{1,2} + \gamma a_{1,1} + \gamma a_1 G_+ (i3\pi/\gamma) \right) \left( \frac{h}{\alpha} \right)^2 \\
+ \frac{3\gamma + \pi}{\alpha\pi(\pi+\gamma)} \tan \frac{\pi\gamma}{\pi-\gamma} G_- \left( -i\frac{\pi}{\gamma} \right) G_+^2 \left( -i\frac{2\pi}{\pi-\gamma} \right) \left( \frac{h}{\alpha} \right)^{6\gamma/(\pi-\gamma)-1} \right\} \] (129)

3.2.3. Isotropic XXZ-point. The isotropic case \( \gamma = 0 \) (i.e. \( \Delta = 1 \)) is treated in the same manner as the anisotropic case \( \gamma \neq 0 \). Therefore, we rescale (80) via \( \lambda_j \rightarrow \gamma \lambda_j \). This is equivalent to substituting \( k \rightarrow k/\gamma \) in Fourier space. Then
\[ \bar{s}(k) = \frac{1}{2 \cosh k/2} \]
\[ \bar{\rho}_0(k) = \bar{s}(k) + \frac{1}{2N} \frac{1}{2 \cosh k/2} \left( 1 + e^{-|k|/2} \right) . \] (130)
Whereas the analyticity properties of the bulk contribution to (130) are qualitatively the same as in (85), the boundary contribution shows, besides poles, a cut along the imaginary axis. The functions $g^{(1,2)}(1,2)$ are determined as in the anisotropic case, where now the integrals in (92), (93) encircle the cuts of (130) and of

$$
\kappa(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-|k|/2}}{2 \cosh k/2} e^{-ikx} dk
$$

(that is the isotropic limit of (87)). Accordingly, the functions $G_\pm$ from equations (95), (96) now read

$$
G_+(k) = \sqrt{2\pi} \left( \frac{(-ik)^{-ik/(2\pi)}}{\Gamma(1/2 + ik/(2\pi))} \right) e^{-iak}
$$

$$
a = -\frac{1}{2\pi} - \frac{\ln(2\pi)}{2\pi}
$$

$$
G_-(k) = G_+(k).
$$

Let us first consider the bulk contribution. We find

$$
\tilde{g}^{(1)}_+(k) + \tilde{g}^{(2)}_+(k) = G_+(k) \left( \frac{a_0}{k + i\pi} e^{-\pi B} \right. - \frac{iG_-(3i\pi)}{k + 3i\pi} e^{-3\pi B} \left. + G_+(k) \begin{cases} 
\frac{\beta_0 e^{-\pi B}}{kB^2}, & k \neq 0 \\
\frac{\beta_1 e^{-\pi B}}{B^2} + \frac{\beta_2 \ln B}{B^2} e^{-\pi B} + \frac{\beta_3 e^{-\pi B}}{B^2}, & k = 0 \end{cases} \right.
$$

with

$$
\beta_0 = \frac{a_0}{16\pi^2} G^2(0) \quad \beta_1 = \frac{a_0}{4\pi^2}
$$

$$
\beta_2 = -\frac{a_0}{8i\pi^3} \quad \beta_3 = \frac{a_0}{8i\pi^3} (-\ln \pi + 1).
$$

Inserting (132) into (107) and performing the maximization (108), one obtains

$$
e^{-\pi B} = \frac{h}{\alpha} \left( 1 + \frac{\alpha_1}{\ln h/\alpha} + \frac{\alpha_2 \ln \ln h/\alpha}{\ln^2 h/\alpha} + \frac{\alpha_3}{\ln^2 h/\alpha} \right)
$$

with

$$
\alpha_1 = -\frac{\beta_1 \pi^2}{a_0} = -\frac{1}{4}
$$

$$
\alpha_2 = \frac{\beta_2 \pi^3}{a_0} = -\frac{1}{8}
$$

$$
\alpha_3 = \frac{\pi^2}{a_0} (i\beta_3 \pi + i\beta_1 - 2\beta_0 - i\beta_2 \ln \pi) = -\frac{1}{8}.
$$

Combining (132), (133) and (107), one obtains for the bulk susceptibility

$$
\chi_{\text{bulk}} = \chi_{\text{bulk}}(h = 0) \left( 1 + \frac{2\alpha_1}{\ln h/\alpha} + \frac{2\alpha_2 \ln \ln h/\alpha}{\ln^2 h/\alpha} + \frac{\alpha_3}{\ln^2 h/\alpha} \right),
$$

\[\text{ doi:10.1088/1742-5468/2006/01/P01007} \]
with $\alpha_4 = 5/16$, $\chi_{\text{bulk}}(h = 0) = J/\pi^2$, and $\alpha = \sqrt{2\pi^3}/e$. We now set $\alpha = h_0 \delta$, where $\delta$ is determined such that the term $\sim \ln^{-2} h/\alpha$ in (134) is absorbed into the $1/\ln(h/h_0)$-term. This prescription fixes the scale uniquely. One finds $\delta = \exp(-5/8)$ and

$$h_0 = \sqrt{2\pi^3} e^{-9/8}.$$  \hfill (135)

Then equation (134) reads

$$\chi_{\text{bulk}} = \frac{1}{J\pi^2} \left( 1 - \frac{1}{2 \ln h/h_0} - \frac{\ln |\ln h/h_0|}{4 \ln^2 h/h_0} \right).$$

Let us now consider the boundary contribution. In (92), the $[\cdots]_+$ bracket yields contributions $O(\exp [-\text{constant} B])$ from the poles, and algebraic contributions due to the cut. The exponential contributions are clearly subleading in comparison to the algebraic ones, so only the latter are calculated in the following. Using the expressions for $G_\pm(k)$, we find (omitting the bulk contribution)

$$\tilde{g}_+^{(1)}(k) = \begin{cases} G_+(0)(\alpha_1/B + \alpha_2(\ln B)/B^2 + \alpha_3/B^3) & \text{for } k = 0 \\ O((\ln B)/B^3, 1/B^3) & \text{for } k \neq 0 \end{cases}$$

$$\alpha_1 = \frac{1}{\sqrt{2\pi}}, \quad \alpha_2 = -\frac{\sqrt{2}}{4\pi^2}, \quad \alpha_3 = \frac{1}{\sqrt{2\pi^2}} \left( \ln 2 - \frac{1}{2} \ln(2\pi) \right).$$

Leading and next-leading contributions are here already contained in $\tilde{g}_+^{(1)}$, so we do not consider further corrections stemming from $\tilde{g}_+^{(2)}$. From (105), (107), (108) we obtain

$$B = \frac{1}{\pi} \ln \frac{h}{\alpha} \quad \text{and} \quad \alpha^{-1} = \frac{G_+(0)}{2\pi JG_+(i\pi)}.$$  \hfill (136) \hfill (137)

These equations are obtained by those from the anisotropic case, (109), (110), by scaling $B \to \gamma B$ and sending $\gamma \to 0$ afterwards. Carrying out the same steps as led to (111b), one finds the boundary contribution

$$s_B^\tilde{\delta}(h) = -\frac{1}{4} \left( \frac{1}{\ln h/h_0} + \frac{\ln |\ln h/h_0|}{2 \ln^2 h/h_0} \right) + o(\ln^{-2} h) \quad \text{and} \quad \chi_B(h) = \frac{1}{4h} \left( \frac{1}{\ln^2 h/h_0} + \frac{\ln |\ln h/h_0|}{\ln^3 h/h_0} - \frac{1}{2 \ln^3 h/h_0} \right) + o \left( \frac{1}{h \ln^3 h} \right) \quad \text{for } T = 0.$$  \hfill (138) \hfill (139)

$$\tilde{h}_0 = \alpha/\sqrt{2} = J\pi \sqrt{\pi/e}.$$  \hfill (140)

The scale $\tilde{h}_0$ has been chosen such that in (138), no terms $O(\ln^{-2} h)$ occur. Note that $\tilde{h}_0 \neq h_0$. The results (139), (140) agree with the TBA work by Frahm et al [23] for $T = 0$. Furthermore, agreement is found with [16, 17, 24], where scales which differ from ours (140) by a constant factor were used.
4. Determining the amplitudes by comparing field theory and the Bethe ansatz

Apart from the amplitudes $\lambda_1, \alpha, \beta$, the bulk and boundary parts of the ground state energy as well as the constant term in the boundary susceptibility have been left unknown in our final field theory result (56) and (57). These quantities have been calculated in the last section using the Bethe ansatz. In terms of the Luttinger parameter $K$ we can write the ground state energy as

$$e_{0}^{\text{bulk}} = -\frac{J}{4}\cos\frac{\pi}{K} - \frac{J}{8\pi}\int_{-\infty}^{\infty} dk \frac{\sin\frac{\pi}{2K} \sinh\frac{\pi}{2K}(K-1)\pi k}{\sinh\frac{\pi k}{2K} \cosh\frac{(K-1)\pi k}{2K}}$$

and

$$E_{0}^{B} = \frac{J}{4} \left( 2 + \cos\frac{\pi}{K} \right) - \frac{J}{8\pi} \sin\frac{\pi}{K} \sinh\frac{\pi}{2K} \int_{-\infty}^{\infty} dk \frac{\cosh\frac{(K-2)\pi k}{4K} \cosh\frac{(K-1)\pi k}{4K}}{\sinh\frac{\pi k}{2K} \cosh\frac{(K-1)\pi k}{4K} \cosh\frac{(K-1)\pi k}{2K}}$$

The constant $B$ in equation (57) can also be expressed in terms of the Luttinger parameter

$$B = \frac{K}{2\pi v^2} \frac{1}{2\sqrt{2}} \cos\frac{\pi}{4K-4}$$

Next we determine the amplitudes. By taking the limit $T \to 0$ of equation (40) we obtain

$$E_{1}^{(1,\text{conv})} = -\lambda_1 K^{2K} \Gamma(-2K) \sin(K\pi) \left( \frac{h}{v} \right)^{2K-1}$$

The amplitude $\lambda_1$ of the umklapp term can now be found by comparing this with the BA result in equation (111b). This leads to

$$\lambda_1 = \frac{K\Gamma(K) \sin\pi/K}{\pi\Gamma(2-K)} \left[ \frac{\Gamma \left( 1 + \frac{1}{2K-2} \right)}{2\sqrt{\pi} \Gamma \left( 1 + \frac{K}{2K-2} \right)} \right]^{2K-2}$$

and agrees with Lukyanov’s result in equation (2.24) of [14] where our amplitude $\lambda_1$ is related to his amplitude $\lambda$ by $\lambda_1 = v\lambda/2\pi$. Here we have determined $\lambda_1$ by comparing with a boundary quantity. We can, of course, also compare the zero-temperature limit of the bulk contribution (47) with (126). This yields the same result, as it should.

The amplitudes of the terms with scaling dimension 4 represent a more subtle problem. From the zero-temperature Bethe ansatz solution (126) we can only obtain the amplitude of the $h^4$-term in the free energy. According to (56), however, this amplitude depends on $\alpha$ and $\beta$. One possibility would be to calculate the amplitude of the $h^2 T^2$-term in $f_{\text{bulk}}$ from a finite temperature BA solution. Although such a solution exists, an analytic formula for this term is difficult to obtain. We therefore follow Lukyanov’s idea for obtaining both amplitudes from the $h^4$-term in $f_{\text{bulk}}$ alone, by using symmetry arguments. The coefficient of the $h^3$-contribution in (126) consists of two terms. The first of these terms

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The open $XXZ$-chain vanishes at the free fermion point due to the tan function. We can identify this term as the one determining the amplitude $\alpha$, because $\alpha$ is associated with a mixing of left- and right-movers and therefore has to vanish at the free fermion point. The other term then determines $\beta$ leading to

$$\alpha = -\pi^2 v \tan \frac{\pi K}{2K-2}$$

and

$$\beta = -\frac{v \pi^2 \Gamma \left(\frac{3K}{2K-2}\right) \Gamma^3 \left(\frac{1}{2K-2}\right)}{6K \Gamma \left(\frac{3}{2K-2}\right) \Gamma^3 \left(\frac{K}{2K-2}\right)}.$$  

These results also agree with Lukyanov’s formula (2.24) in [14] with $\alpha = -2\pi^3 v \lambda_+$ and $\beta = -2\pi^3 v \lambda_-.$

### 5. Divergent amplitudes and logarithmic corrections

From (56) and (57) the bulk and boundary susceptibilities for zero magnetic field can be derived by taking derivatives with respect to $h$ leading to

$$\chi_{\text{bulk}}(T, h = 0) = \frac{K}{2\pi v} - (\alpha + 6\beta) \frac{KT^2}{24\pi^2 v^4} + \frac{\lambda_1^2}{32\pi v^3} \Gamma^2(1/2 - K)$$

$$\times \Gamma^2(1 + K) \sin(2\pi K) \left[\Psi'(1 - K) - \Psi'(K)\right] \left(\frac{\pi T}{v}\right)^{4K-4},$$

and

$$\chi_B(T, h = 0) = 2B - \alpha \frac{KT}{4\pi^3 v^3} + \lambda_1 \frac{K T \Gamma(K) \Gamma(3 - 2K) \left(\pi^2 - 2\Psi'(K)\right)}{2v^2 \Gamma(2 - K) \Gamma(2 - K)} \left(\frac{2\pi T}{v}\right)^{2K-3}. \tag{149}$$

Interestingly, the constant term $2B$ is closely related to the constant in the bulk susceptibility (see (143)). The two terms become equivalent at the free fermion point as expected from the calculations in section 2.3. On the other hand, for $T = 0$, bulk and boundary susceptibilities are given in equations (128), (129).

For certain anisotropies, terms in $\chi(T = 0, h)$ and $\chi(T, h = 0)$ show divergences. In this section, we will show that these divergences cancel and give rise to logarithmic corrections. In the first part, we will focus on $\chi(T = 0, h)$, whereas in the second part, $\chi(T, h = 0)$ is treated. In order to keep contact with the notation introduced in sections 2 and 3, we will write our results in terms of $\gamma = \arccos \Delta$ for the $T = 0$ case, whereas $K = \pi/(\pi - \gamma)$ will be employed for $h = 0$ at finite $T$.

#### 5.1. Logarithmic corrections in $\chi(T = 0, h)$

Let us come back to the enumeration of poles encountered within the Wiener–Hopf procedure in the leading and next-leading orders, equations (98), (99), (112). Combining the relation $B = B(h)$, equation (109), with the functional dependence of the energy on $4$ This does not come as a surprise: this term has been obtained from the second bracket in (93). However, at the free fermion point $\gamma = \pi/2$, the integration kernel $\kappa$ vanishes identically, $\kappa|_{\gamma=\pi/2} \equiv 0$. 

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\( \tilde{g}_+ \), equation (107), we can read off the exponents of \( h \) dependent contributions. Namely, the poles (98) lead to terms

\[ \sim h^{2n}, \quad n = 0, 1, \ldots \]  

(150)

both in the boundary and the bulk susceptibility. Furthermore, the \( k_m^{(2)} \) from (99) lead to contributions

\[ \sim h^{(\gamma(4m+3)-\pi)/(\pi-\gamma)}, \quad m = 0, 1, \ldots \]  

(151)

in the boundary part. As far as the next-leading order is concerned, one determines the exponents to the bulk susceptibility due to the second term in (93) from the combination of poles (98), (112). This results in terms

\[ \sim h^{2(n+2m+1)} + h^{2(n+2(\gamma/\pi-\gamma)l)}, \quad n, m = 0, 1, \ldots; \quad l = 1, \ldots \]  

(152)

The next-leading order of the boundary susceptibility shows, apart from terms similar to (152), additional contributions of the form

\[ \sim h^{4n+1+(2\gamma/(\pi-\gamma))(2m+1)} + h^{(2\gamma/(\pi-\gamma))(2m+1+2l)-1}, \quad n, m = 0, 1, \ldots; \quad l = 1, \ldots \]  

(153)

which result from combining (99) with (98) and (112). Note that the pre-factors of the leading terms in equations (150), (151), (152), (153) are those which have been determined in section 3. By carrying out the Wiener–Hopf procedure to higher orders, it would be possible to obtain further pre-factors, at the expense of more and more cumbersome calculations.

The enumeration of possible exponents in (150), (151), (152), (153) is far from complete. These exponents have been found from extrapolating the first-and second-order results of the perturbation expansion of \( \tilde{g}_+ \), while using the first-order result (109) and the leading orders in (107). In higher orders of the \( \tilde{g}_+ \) expansion, these exponents mix with each other and further orders appear.

So far, we excluded the double poles in equation (100), which occur when two poles of the types (98), (99) coincide, that is, when exponents stemming from (150), (151) cross. Again combining equations (109), (107) we obtain logarithmic contributions

\[ \sim h^{2n \ln h}, \quad n = 0, 1, \ldots \]  

(154)

to the boundary susceptibility. The same happens if exponents in the next-leading order contributions cross, therefore yielding logarithmic contributions of the form (154), with \( n \geq 1 \) there, for both the bulk and the boundary. In order to obtain the coefficient of the logarithmic terms, it suffices to know the amplitudes of the terms whose exponents cross: they show divergences at the crossover points, which cancel to yield the logarithms.

Consider the constant term in \( \chi_B(h) \); cf equation (129). It displays poles at

\[ \gamma_n = \frac{\pi}{4n+3} \]  

(155)

with an accumulation point at \( \gamma = 0 \), whereas the coefficient of the \( h \) dependent contribution with exponent \( 2\gamma/(\pi-\gamma) - 1 \) has poles at

\[ \gamma_m = \frac{2m+1}{2m+3\pi} \]  

(156)

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with an accumulation point at $\gamma = \pi$. Obviously, $\gamma_n = \gamma_m$ for $n = 0 = m$, which means $\gamma_0 = \pi/3$ (the case $n = m = -1$, $\gamma_{-1} = \pi$, is excluded here). On setting $\gamma = \pi/3 + \epsilon$ and expanding in $\epsilon$, the two divergences cancel and one obtains

$$\chi_B(h)|_{\gamma=\pi/3} = -\frac{1}{\sqrt{3}\pi^2} \ln \left( \frac{he^{3-\pi/2}}{4\pi^{3/2}} \right).$$

(157)

As far as the other poles (155), (156) are concerned, note that they coincide with (100) for $m = 0$ or $n = 0$ there, respectively. This means that we expect higher order terms, whose coefficients show poles at (155), such that logarithms of the form (154) occur, with $n \geq 1$ there.

A similar crossover at $\gamma = \pi/3$ happens in the bulk part in the next-leading order, when the exponents $2, 4\gamma/(\pi - \gamma)$ cross in equation (128). Again divergences in the two corresponding amplitudes cancel, as can be seen by expanding $\gamma = \pi/3 + \epsilon$. Then one finds

$$\chi_{\text{bulk}}|_{\gamma=\pi/3}(h) = \frac{1}{\sqrt{3}\pi} - \frac{2}{3\sqrt{3}\pi^3} h^2 \ln \frac{he^{-1/3}}{4\pi^{3/2}}.$$ 

(158)

Finally, let us consider the additional crossover in the next-leading order of $\chi_B(h)$. In equation (129), three exponents have been identified: 0, $2\gamma/(\pi - \gamma) - 1$, 2. Contrary to the bulk case, there are now two crossover points: $\gamma = \pi/3$ and $\gamma = 3\pi/5$. At $\gamma = \pi/3$, the (leading) logarithmic contribution has been identified in equation (157). At $\gamma = 3\pi/5$, a (next-leading) logarithmic contribution appears, which is

$$\chi_B(h) = \chi_0 \left( 1 + h^2 \left( \frac{135}{64} \frac{(3 + \sqrt{5})\Gamma^2(4/3)}{\pi^{3/2}(3 + \sqrt{5})(5 + 2\sqrt{5})\Gamma^3(11/6)} \right. \right.$$ 

$$\times \left( -18 \ln h - 31 + 39 \ln 2 + 9 \ln \frac{(5 + \sqrt{5})\Gamma^2(11/6)}{\Gamma^2(1/3)} \right)$$

$$\left. + \frac{405}{64} \frac{(2 + \sqrt{3})(3 + \sqrt{5})\Gamma^3(4/3)}{(3 + \sqrt{5})\pi^{1/2}(5 + 2\sqrt{5})\Gamma^3(11/6)} - \frac{27}{10} \frac{(1 + \sqrt{3})(3 + \sqrt{5})}{\pi(3 + \sqrt{3})(5 + 2\sqrt{5})} \right)$$

(159)

with

$$\chi_0 = \frac{403 + \sqrt{3}}{\pi^{1/2}(5 + 2\sqrt{5})(5 + \sqrt{5})^{-7/2}}.$$ 

(160)

This completes our discussion of the leading and next-leading terms in the susceptibilities on the basis of the Bethe ansatz solution at $T = 0$ for the anisotropic XXZ case.

5.2. Logarithmic corrections in $\chi(T, h = 0)$

Let us start our discussion for finite temperatures with the bulk susceptibility. The $T^2$-term in $\chi_{\text{bulk}}$ contains the amplitude $\alpha$ which is defined in (146). $\alpha$ is divergent for $K = (2n + 1)/2n$ with $n = 1, 2, \ldots$.\footnote{The amplitude $\beta$ does not show any divergences.} Obviously $\chi_{\text{bulk}}$ does not diverge at these points so this divergence has to be cancelled by other divergent terms. In fact, the $T^{4K-4}$-term

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also has divergences at $K = (2m + 1)/2$ with $m = 1, 2, \ldots$ due to the $\Gamma^2(1/2 - K)$-factor. The only point where the two terms diverge simultaneously is therefore $K = 3/2$ and we will show that these divergences indeed cancel each other here and lead to a logarithmic correction. But what happens to the other divergences? Let us first consider the divergences in the $T^{4K-4}$-term. At $K = (2m + 1)/2$ the temperature dependence becomes $T^{4n-2} = T^2, T^6, T^{10}, \ldots$. Terms like $h^2T^6, h^2T^{10}, \ldots$ appear in the free energy in perturbation theory in the irrelevant terms with integer scaling dimension. For example, in $n$th-order perturbation theory in the $(\partial_x^4 \phi)^4$ operator we will get a $h^2T^{4n-2}$-term. These higher order corrections will interfere with the $T^{4K-4}$-term and cancel the divergences at $K = (2m+1)/2$. The result will be a $T^{4n-2}\ln T$ behaviour at these points. As the $T^2$-term dominates for $K > 2$ these are just logarithmic corrections in next-leading contributions.

Much more interesting are the divergences at $K = (2n+1)/2n$ in the $T^2$-term. They yield $T^2\ln T$-terms and the points where this happens become dense for $K \to 1$ ($\Delta \to 1$). The divergence at $K = 3/2$ in the $T^2$-term is cancelled by the divergence in the $T^{4K-4}$-term. In general, the divergence at $K = (2n+1)/2n$ is cancelled by a $T^{4nK-4n}$-term which one obtains in $n$th-order perturbation theory in the $\cos(2\phi/R)$-operator.

The only case where we can give an explicit result for the logarithmic term is $K = 3/2$. Here we find

$$\chi_{\text{bulk}}(T, h = 0) = \frac{1}{\sqrt{3\pi}} + \frac{142 + 24\gamma + 12\ln(3888) - 21\zeta(3)}{243\sqrt{3\pi}}T^2 - \frac{8}{81\sqrt{3\pi}}T^2\ln T, \quad (161)$$

where $\gamma$ is Euler’s constant and $\zeta(x)$ Riemann’s zeta function.

In the boundary susceptibility similar things happen. Here even the constant term (143) as determined using the BA shows divergences at $K = (4n-1)/(4n-2) = 3/2, 7/6, \ldots$ due to the $\cos$ term in the denominator, see also equation (155). The $T^{2K-3}$-term, on the other hand, has a divergent amplitude for $K = (2n+1)/2$. Again all these divergences have to cancel each other to logarithmic corrections. For $K = 3/2$ we can derive an explicit result

$$\chi_{B}(T, h = 0) = \frac{-6 + 4\gamma + 2\pi + 2\ln(3888) - 7\zeta(3)}{4\sqrt{3\pi}^2} - \frac{\ln T}{\sqrt{3\pi}^2} + \mathcal{O}(T\ln T). \quad (162)$$

Here the $T\ln T$-term stems from the term linear in $T$ whose amplitude also diverges at $K = 3/2$.

We summarize our results in figure 1.

6. Comparison with numerical results

To check our analytical formulae, in particular those for the boundary susceptibility, we use numerical data. For $T = 0$ we have solved equation (83) numerically (for more details see [11]). This allows us to obtain $\chi_B(h)$ and to compare with the analytical formula (129) if $|h| \ll \alpha$. Such a comparison has already been performed in [11] for the repulsive regime $0 \leq \Delta \leq 1$, verifying our analytical result for the constant term and for the term which involves a fractional power of $h$. These are the dominant contributions for $1 < K < 5/2$. For $K > 5/2$ the leading term is quadratic in $h$. To check this term also we present in figure 2 numerical data in the attractive regime. Another point worth checking is the two anisotropies $K = 3/2$ and $K = 5/2$ where we have obtained the explicit formulae (157)
Figure 1. Crossover of critical exponents, depending on the anisotropy $\Delta$, in the leading orders. Black lines are those exponents which occur both in the bulk and boundary susceptibilities (namely 0 and 2). The leading non-integer exponent in the boundary contribution is dashed blue ($2K - 3$), the one in the bulk contribution dotted blue ($4K - 4$). Green is the exponent 1, which only occurs at finite $T$ in the boundary contribution. All crossover points are denoted by circles. The crossover between 1 and $2K - 3$ at $\Delta = 0$ has no consequences, since the corresponding amplitudes vanish. At all other crossover points, logarithmic corrections appear. The vertical lines denote $\Delta = (1 - \sqrt{5})/4 (\gamma = 3\pi/5)$, $\Delta = 0$ and $\Delta = 0.5$.

and (159) for the logarithmic corrections. These are compared with numerical data in figures 3 and 4, respectively. Next, we turn to finite temperatures. The bulk quantities can be calculated numerically on the basis of the Bethe ansatz solution in the quantum transfer matrix approach [7]. Comparison between these data and equation (148) for the repulsive and for the attractive regime are shown in figures 5 and 6, respectively. Figures 5(b) and 6(b) show $\chi(T, h = 0) - \chi(T = 0, h = 0)$ in double-logarithmic plots. Excellent agreement is found for both the amplitudes and the exponents of the leading $T$-corrections, thus confirming (148) first derived by Lukyanov [14]. In particular, note the dependence of the exponent of the leading $T$-correction on the anisotropy in the repulsive regime (figure 5(b)), whereas this exponent is constant in the attractive regime (figure 6(b)).

For the boundary susceptibility at finite temperature no Bethe ansatz solution is known today. We have therefore calculated this quantity by using the density matrix renormalization group applied to transfer matrices (TMRG). This method is particularly suited because the thermodynamic limit can be taken exactly and no finite size corrections disguise the boundary contributions we are looking for. This method has already been used in [11] to obtain data for the repulsive regime and the reader is referred to this paper for more details about the TMRG. In figure 7 we show data for the boundary susceptibility in the attractive regime. Interestingly, $\chi_B$ first decreases when starting from infinite temperature down to a temperature $T_0$ which depends on anisotropy before it starts increasing at lower temperatures. This behaviour can be understood in terms of a crossover from antiferromagnetic to ferromagnetic short range order in the bulk with increasing temperature, as studied in [25]. According to [25], a change in the
Figure 2. (a) Boundary susceptibility $\chi_B(h)$: comparison between a numerical solution of the BA equations (black solid lines) and the analytical solution for $h/J \ll \alpha$ in the attractive regime (blue dotted lines). (b) The difference $\chi_B(h) - \chi_B(0)$ on a double-logarithmic scale. For $\Delta < \cos(3\pi/5) \approx -0.31$, the leading $h$-term has constant exponent 2, whereas for $\Delta > \cos(3\pi/5)$, the exponent depends on $\gamma$, according to equation (129).

Figure 3. Numerical data for the boundary susceptibility (black solid line) at $K=3/2$ (i.e. $\gamma = \pi/3$) compared to formula (157) (blue dotted line). The inset shows $\chi_B(h) - c \ln h$, where $c = -1/\sqrt{3\pi^2}$. According to equation (157), this yields the scale of the logarithmic divergence.

dispersion relation of elementary excitations from linear to quadratic behaviour occurs when increasing the temperature from $T < T_0(\gamma)$ to $T > T_0(\gamma)$. Note that the critical temperature $T_0(\gamma)$ depends on the anisotropy.

We expect the temperature of crossover between these two regimes to be described by the same formula for $T_0(\gamma)$ as for the bulk, which reads [25]

$$T_0(\gamma) = A \frac{\sin \gamma}{\gamma} \tan \frac{\pi(\pi - \gamma)}{2\gamma}. \quad (163)$$

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Figure 4. Numerical data for the boundary susceptibility (black solid line) at $K = 5/2$ (i.e. $\gamma = 3\pi/5$) compared to formula (157) (blue dotted line). For the plot in the inset, the constant $\chi_B(h=0)$ has been subtracted. Note the double-logarithmic scale in the inset.

Figure 5. Comparison between numerical data (black solid lines) for the bulk susceptibility in the repulsive regime and formula (148) (blue dotted lines) for $\gamma = 0.5, 0.8, \pi/3, 1.3$, corresponding to $\Delta = 0.88, 0.7, 1/2, 0.27$ (from bottom to top in (a) and from top to bottom in (b), (c)). In (b), the constant $\chi(T=0, h=0)$ has been subtracted; the inset (c) is a zoom of (b).

Here $A$ is determined by a matrix element which is different for boundary and bulk susceptibilities. This matrix element cannot be calculated using the BA. In the inset of figure 7 we show that this formula does indeed describe very well the minima which occur in $\chi_B$ where $A$ is obtained from a fit.

Finally, we have a closer look at the low temperature regime of figure 7 and compare the TMRG data with (149). Figure 8 shows excellent agreement, confirming that $\chi_B$ depends linearly on temperature in the attractive regime for $T \ll 1$.
Figure 6. Comparison between numerical data (black solid lines) for the bulk susceptibility in the attractive regime and formula (148) (blue dotted lines) for $\gamma = \pi - 0.5, \pi - 0.8, 2\pi/3, \pi - 1.3$, corresponding to $\Delta = -0.88, -0.7, -1/2, -0.27$ (from top to bottom in (a) and (b)). In (b), the constant $\chi(T = 0, h = 0)$ has been subtracted.

Figure 7. TMRG data for $\chi_B(T)$ in the attractive regime. The black diamonds represent the zero-temperature result known from the BA. The black dots denote the minima $T_0$ of $\chi_B(T)$. In the inset we show that these minima (black dots) are well described by formula (163) (red dots) with $A = 1.245$ obtained from a fit. The dashed lines are a guide to the eye.

7. Conclusions

We have studied low energy thermodynamic and ground state properties of the open spin-$1/2$ XXZ-chain by combining the bosonization technique with the exact Bethe ansatz solution in the critical regime $-1 < \Delta < 1$. Bosonization has allowed us to obtain a low temperature, low field expansion of the free energy in terms of $T, h$ for both the bulk and the boundary parts of the free energy with unknown coefficients. We have argued
that the coefficients of the regular terms in the boundary part (these are those powers of $h, T$ which appear also in the bulk part) involve the short distance lattice cut-off and therefore cannot be obtained from field theory. All leading terms in the bulk part, on the other hand, are cut-off independent and their coefficients could be determined from the Bethe ansatz by expanding the ground state energy in terms of the magnetic field $h$.

For the boundary free energy only the coefficients of two terms turned out to be cut-off independent. These are an $h^2T$- and an $h^2T^2K^{-3}$-term. Fortunately, these two terms combined with an $h^2$-term obtained using the BA give a complete low energy description of the boundary susceptibility $\chi_B$ for all anisotropies.

We used the Wiener–Hopf procedure within the Bethe ansatz in the thermodynamic limit to obtain the ground state energy and a systematic low field expansion of the susceptibility at zero temperature. The coefficients of the leading and next-leading terms in this expansion have been calculated explicitly for both the bulk and the boundary contributions. The possible exponents of higher order terms have been classified in a systematic way.

We compared our results with numerical data obtained by various techniques: the $T = 0$ Bethe ansatz equations involved solving linear integral equations numerically, the behaviour at finite $T$ of the bulk susceptibility was calculated in the quantum transfer matrix approach, and the behaviour at finite $T$ of the boundary susceptibility was obtained from the density matrix renormalization group applied to transfer matrices. In all cases, we found excellent agreement between analytical and numerical results.

We identified several crossover phenomena. Depending on the anisotropy, the crossover of scaling dimensions of the irrelevant operators in the low energy effective Hamiltonian leads to a crossover of critical exponents of $T, h$ in the free energy. Associated with this crossover are divergences in the corresponding amplitudes, which cancel to yield contributions logarithmic in $T, h$ at the crossover points. Whereas this happens

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6 There are also higher powers in $h, T$ which will be cut-off independent, but those terms are not very helpful because they are next-leading compared to a term with unknown coefficient.
in the next-leading orders in the bulk, this affects the boundary contributions both in leading and in next-leading orders. Furthermore, we observed a crossover in the boundary susceptibility in the attractive regime, due to competing antiferromagnetic or ferromagnetic ordering tendencies at low and high temperatures, respectively.

We think that the rich results for the boundary behaviour analysed in this paper will stimulate further research in the direction of an exact treatment of the boundary free energy at finite temperatures.

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