Boundary contributions to specific heat and susceptibility in the spin-1/2 XXZ chain

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Exact low-temperature asymptotic behavior of boundary contribution to specific heat and susceptibility in the one-dimensional spin-1/2 XXZ model with exchange anisotropy $1/2 < \Delta \leq 1$ is analytically obtained using the Abelian bosonization method. The boundary spin susceptibility is divergent in the low-temperature limit. This singular behavior is caused by the first-order contribution of a bulk leading irrelevant operator to boundary free energy. The result is confirmed by numerical simulations of finite-size systems. The anomalous boundary contributions in the spin isotropic case are universal.

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Irrelevant operators in the renormalization-group (RG) theory are considered to give only subleading contributions to any physical quantity by definition. A subtle exception to this general rule can be found, however, when a bulk irrelevant operator has not so large boundary scaling dimension. Consider, for example, a Gaussian theory in (1+1)-dimension with a bulk perturbing operator $O$ having scaling dimension, $x_o$, larger than 2. First, let us impose periodic boundary condition to a one-dimensional (1D) system of length $L$. In second-order perturbation the irrelevant operator is found to give a contribution of order $L^2 x_o^{-3}$ to the specific heat of the periodic system at temperature $T$. This is small compared with the leading term of order $LT$.

The lattice constant is unity. The bosonic field, $\phi$, is boundary scaling dimension of the perturbing operator. If $2 < x_o' < 3$, then the boundary specific heat gives a dominant contribution at low enough temperatures, even though the operator is irrelevant.

This interesting possibility is in fact realized in the 1D spin-1/2 XXZ model, as recently pointed out by Fujimoto. The model with open boundaries was studied earlier by de Sa and Tsvelik using Bethe ansatz who found anomalous boundary contributions to the specific heat and spin susceptibility. Similar and more extensive calculations for the spin isotropic case have shown that the boundary contribution to the spin susceptibility at $T = 0$ exhibits a Curie-like behavior with a logarithmic correction as a function of a weak external field. These results seemed somewhat mysterious, as irrelevant operators localized at a boundary can give at most a temperature-independent contribution to the susceptibility. The origin of these anomalous boundary contributions was not understood, until Fujimoto and Eggert recently examined boundary contributions from a bulk leading irrelevant operator to the specific heat and the susceptibility. Their theory seems rather complicated, however, as it uses properties of boundary states in the boundary conformal field theory. The aim of this paper is to present an alternative, simpler, and straightforward derivation of the exact results using the Abelian bosonization method. We also verify our analytical results with numerical calculations for the anisotropic XXZ model.

Our results are relevant to many 1D correlated electron systems with impurities. An impurity potential in a 1D system of repulsively interacting electrons is strongly renormalized and becomes perfectly reflecting in the low-energy limit. A long wire with a finite density of impurities is thus effectively cut into many pieces of finite length. Measurements of the specific heat and the susceptibility of such a wire will exhibit the anomalously large boundary contributions.

We analyze the spin-1/2 XXZ model in a weak magnetic field,

$$H = J \sum_{j=1}^{L} \left( S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right) - h \sum_{j=1}^{L} S_j^z,$$

where $J > 0$ and $L$ is the number of sites. We are interested in the case where the exchange anisotropy $\Delta$ is in the parameter range

$$\frac{1}{2} < \Delta \leq 1,$$

for which we shall find an anomalous contribution to the boundary free energy.

First we consider a semi-infinite spin chain, taking the limit $L \to \infty$. Its free energy has, in addition to a bulk term, a boundary term of order 1 due to the presence of the boundary at $j = 1$. We calculate the boundary free energy at low temperatures using the low-energy effective theory for the Hamiltonian, which is the Gaussian model perturbed by a nonlinear operator. The Hamiltonian density of the effective theory is

$$H = \frac{\nu}{2} \left[ \left( \frac{d\phi}{dx} \right)^2 + \Pi^2 \right] + \lambda \cos \left( \frac{2\phi}{R} \right) - \frac{h}{2\pi R} \frac{d\phi}{dx}.$$

The lattice constant is unity. The bosonic field $\phi(x)$ and its conjugate operator $\Pi(x)$, defined on the positive half
Under the boundary condition (8) the bosonic field can be expanded as

$$v = \frac{\sin(\pi\eta)}{2(1 - \eta)},$$

with which the spin velocity $v$ at $h = 0$ is written,

$$v = \frac{\sin(\pi\eta)}{2(1 - \eta)}. \tag{5}$$

We note that in the parameter range [2] of our interest $\eta$ satisfies the inequality

$$\frac{2}{3} < \eta \leq 1 \tag{6}$$

at $h = 0$. The original spin operator can be expressed with the fields $\phi$ and $\Pi$. In particular, $S_j^z$ is written as

$$S_j^z = \frac{1}{2\pi R} \frac{d\phi}{dx} (-1)^j a \sin \frac{\phi(x)}{R}, \tag{7}$$

where $x = j$ and $a$ is a constant calculated in Refs. [13] and [14]. For the semi-infinite wire the bosonic field obeys the boundary condition at $x = 0$:

$$\phi(x = 0) = 0. \tag{8}$$

Once Eqs. (7) and (8) are given, sign of the coupling constant $\lambda$ of the nonlinear operator is fixed to be positive. For the gapless regime ($-1 < \Delta \leq 1$) of the XXZ chain the exact value of $\lambda$ is known to be [13,15].

$$\frac{\lambda}{v} = -2 \sin \left( \frac{\pi}{\eta} \right) \left[ \frac{\Gamma(\frac{1}{2})}{\pi} \right]^2 \left[ \frac{\Gamma(1 + \frac{\eta}{2 - 2\eta})}{2\sqrt{\pi} \Gamma(1 + \frac{\eta}{2 - 2\eta})} \right]^{-2} \tag{9}$$

Under the regularization condition on the zero-temperature correlator in the Gaussian model,

$$\langle e^{i\mu\phi(x)} e^{-i\mu\phi(y)} \rangle = |x - y|^{-\mu^2/2\pi}, \quad x, y, |x - y| \gg 1. \tag{10}$$

We are now ready to calculate the leading contribution to the boundary free energy. We begin with the path integral representation of the partition function $Z$,

$$Z = \int \mathcal{D}\phi \exp \left( -\int_0^{1/T} d\tau \int_0^\infty dx L \right), \tag{11}$$

where the Lagrangian density in the imaginary time is

$$L = \frac{v}{2} \left[ \frac{(\partial \phi)}{(\partial x)} \right]^2 + \frac{1}{v^2} \left[ \frac{(\partial \phi)}{(\partial \tau)} \right]^2 + \frac{\lambda}{R} \cos \left( \frac{2\phi}{R} \right) - \frac{h}{2\pi R} \frac{\partial \phi}{\partial x}. \tag{12}$$

To eliminate the last term ($\propto h$), we change the field as

$$\phi(x, \tau) \rightarrow \phi(x, \tau) + \frac{hx}{2\pi R v}, \tag{13}$$

which yields a constant contribution $-\chi_0 h^2/2$ to the bulk free energy with the bulk susceptibility given by $\chi_0 = L/(2\pi n v)$. This term is not of our main interest and will be discarded in the following analysis.

Since the operator $\lambda \cos(2\phi/R)$ is an irrelevant perturbation in the gapless phase, the low-temperature expansion of the free energy can be obtained by expanding the partition function in powers of $\lambda$. The leading boundary contribution to the free energy then comes from the first-order term $\propto \lambda$ in the expansion. After making the shift [13], the first-order term reads

$$Z_1 = -\lambda \int \mathcal{D}\phi \int_0^{1/T} d\tau \int_0^\infty dx \cos \left( \frac{2\phi}{R} + \frac{2hx}{nv} \right) \exp \left\{ -\frac{v}{2} \int_0^{1/T} d\tau \int_0^\infty dx \left[ \left( \frac{\partial \phi}{\partial x} \right)^2 + \frac{1}{v^2} \left( \frac{\partial \phi}{\partial \tau} \right)^2 \right] \right\}. \tag{14}$$

Under the boundary condition (8) the bosonic field can be expanded as

$$\phi(x, \tau) = \sqrt{\frac{2T}{\pi}} \sum_{n \in \mathbb{Z}} \int_0^\infty dk e^{-i\omega_n \tau} \sin(kx) \phi(k, i\omega_n), \tag{15}$$

where $\omega_n = 2\pi n T$. Inserting the mode expansion (15) into Eq. (14) and performing the Gaussian integral of $\hat{\phi}$, we obtain

$$Z_1 = -Z_0 \frac{\lambda}{T} \int_0^\infty dx \cos \left( \frac{2hx}{nv} \right) \exp \left( -\frac{8T}{nv} \sum_{n \in \mathbb{Z}} \int_0^\infty dk \frac{e^{-|\omega_n|/\Lambda} \sin^2(kx)}{k^2 + (\omega_n/v)^2} \right), \tag{16}$$

where $Z_0 = Z|_{\lambda=0}$ and we have introduced the high-energy cutoff $e^{-|\omega_n|/\Lambda}$ with $\Lambda = v$ to meet the condition (10). The integral and summation in the exponent can be easily performed, leading to the first-order contribution
to the free energy \( F = -T \ln Z \), which is nothing but the leading term in the boundary free energy,

\[
F_1 = \lambda \left( \frac{2\pi T}{v} \right)^{2/\eta} \int_{\alpha}^{\infty} \frac{dx}{\sinh \left( \frac{2\pi T x}{v} \right)^{2/\eta}},
\]

where \( \alpha \) is a short-distance cutoff of the order of half a lattice spacing. Note that \( F_1 \) has a contribution only from the boundary region within the distance \( v/2\pi T \) from the edge of the spin chain. The exponent \( 2/\eta \) is the boundary scaling dimension of the irrelevant operator \( \cos(2\phi/R) \).

Our next task is to evaluate the boundary free energy \( F_1 \) at low temperatures. Let us first consider the simplest case \( b = 0 \). To obtain the low-temperature expansion of the integral in Eq. (17), we change the variable as

\[
\psi = \frac{v}{2\pi T \alpha},
\]

and the boundary contribution to the specific heat is

\[
\varphi/R
\]

where we have set \( \alpha = 0 \) in the convergent integral. The integral in the right-hand side is elementary. After some algebra we find

\[
\int_{0}^{\infty} \frac{x^2 dx}{(\sinh x)^{2/\eta}} = \frac{2^{3/2-4\eta} \eta \Gamma(\frac{1}{\eta}) \Gamma(3-\frac{2}{\eta})}{4 \eta^2 (2-\frac{1}{\eta}) \Gamma(2-\frac{1}{\eta})} \left( \frac{2\pi T}{v} \right)^{\frac{3}{2}-}\eta, \tag{25}
\]

This is the exact leading contribution to the susceptibility in the XXZ chain with \( 1/2 < \Delta < 1 \). Note that \( \chi \) is diverging as \( T \to 0 \). For \( \Delta < 1/2 \) the leading term in the susceptibility is independent of temperature. A logarithmic correction shows up at \( \Delta = 1/2 \).

At \( T = 0 \) the boundary energy \( E_1 \) becomes

\[
E_1 = \lambda \int_{\alpha}^{\infty} \frac{x_0 \cos \left( \frac{2\pi x_0}{\eta v} \right)}{(2\pi x_0)^{2/\eta}} = \frac{\lambda \Gamma(\frac{1}{\eta}) \Gamma(3-\frac{2}{\eta})}{2^{\frac{4}{\eta}-1} \eta} \left( \frac{2\pi T}{v} \right)^{\frac{3}{2}-}\eta - \frac{\lambda \Gamma(3-\frac{2}{\eta}) \sin(\pi(\frac{1}{\eta} - 1))}{4(\frac{2}{\eta} - 1)(\frac{1}{\eta} - 1)} \left( \frac{h}{\eta v} \right)^{\frac{3}{2}-}\eta, \tag{26}
\]

from which we obtain the boundary contribution to the total magnetization

\[
M_b = -\frac{\partial E_1}{\partial h} = \frac{\pi \lambda}{4 \eta v} \Gamma(\frac{3-\frac{2}{\eta}}{\eta}) \left( \frac{h}{\eta v} \right)^{\frac{3}{2}-}\eta, \tag{27}
\]

where higher-order terms \( O(h) \) are ignored. This is the exact form of the leading term in the XXZ chain for \( 1/2 < \Delta < 1 \). The leading terms in \( C_b(T) \), \( \chi_b(T) \), and \( M_b(h) \) we calculated above are found in agreement with those obtained independently by Fujimoto and Eggert, after some analytical transformations are made in their results.

At the isotropic antiferromagnetic Heisenberg point \( (\Delta = 1) \), we cannot substitute \( \lambda \) of Eq. (19) into Eqs. (22), (25), and (27), as it vanishes at \( \eta = 1 \). To circumvent this difficulty, we adapt a RG improved perturbation theory in which we replace a constant \( \lambda \) with a running coupling constant \( \lambda(E) \) at energy scale \( E \). At \( h = 0 \), the
one-loop scaling equations for the sine-Gordon Hamiltonian are given by

\[
\frac{dg}{dl} = \left(2 - \frac{1}{\pi R^2}\right) g, \quad \frac{dR}{dl} = \frac{\pi g^2}{2 R},
\]

(28)

where \( g = \lambda/v \) and \( dl = -d\ln E \). The coupling \( g \) is marginally irrelevant at \( R = 1/\sqrt{2\pi} \) (i.e., at \( \Delta = 1 \)) and decreases to zero logarithmically. To see this explicitly, we may write \( \sqrt{2\pi R} = 1 - \epsilon \) and expand the RG equations (28) in lowest order in \( \epsilon \). We solve the simplified RG equations to find the solution corresponding to the antiferromagnetic Heisenberg chain,

\[
\frac{\lambda(l)}{v} = \frac{1}{2\pi l}, \quad R(l) = \frac{1}{\sqrt{2\pi}} \left(1 - \frac{1}{4l}\right)
\]

(29)

for \( l \gg 1 \). To obtain the leading term in \( C_b(T), \chi_b(T), \) and \( M_b(h) \), we may substitute \( \eta = 1 \) and

\[
\lambda(T, h) = \frac{v}{2\pi \ln \left(\frac{1}{\text{max}(T, h)}\right)}
\]

(30)

into the analytic formulas of the boundary free energy we obtained for \( 1/2 < \Delta < 1 \). For example, the boundary entropy \( S_b \) is found from Eq. (21) to be

\[
S_b = \frac{\pi \lambda(T)}{2v} = \frac{1}{4\ln(T_0/T)},
\]

(31)

from which the boundary specific heat becomes

\[
C_b = \frac{1}{4(\ln(T_0/T))^2},
\]

(32)

in agreement with Ref. [10]. Here \( T_0 \) is a constant of order \( J \). The boundary contribution to the susceptibility is obtained from Eq. (25) as

\[
\chi_b = \frac{\lambda(T)}{8\pi vT} \left[\pi^2 - 2\psi'(1)\right] = \frac{1}{24T \ln(T_0/T)}.
\]

(33)

This result was confirmed later by the corrected calculation in Ref. [10]. The boundary contribution to the magnetization at zero temperature is found from Eq. (24) to be

\[
M_b = \frac{\pi \lambda(h)}{4v} = \frac{1}{8\ln(h_0/h)}
\]

(34)

in agreement with the exact result from the Bethe ansatz. Here \( h_0 \) is another constant of order \( J \). We note that there exist subleading terms to these formulas which are reduced only by a factor of \( 1/\ln(T_0/T) \) or \( 1/\ln(h_0/h) \). Even though they are important for quantitative analysis, we do not try to evaluate it here, as it is beyond the scope of this paper.

Finally, we present comparison between the analytic result of Eq. (28) and numerical data of energy eigenvalues of the XXZ spin chains with open boundaries. Using the density-matrix renormalization-group (DMRG) method, we have computed the lowest energy \( E(L, m) \) of \( H_0 \) in the subspace of the magnetization per site \( m = (1/L) \sum_{j=1}^{L} S_j^z \). The maximum system size we calculated is \( L = 800 \). The number of block states kept in the DMRG calculation is up to 200. The numerical errors due to the DMRG truncation, estimated from the difference between the data with 150 and 200 states kept, are typically less than \( 10^{-5} \). The numerical data are therefore accurate enough for the discussion below.

The energy \( E(L, m) \) is known to depend on the system...
FIG. 3: $\varepsilon_1(m)$ as functions of $(2\pi m)^2$ for typical values of $\Delta$. The curves are the fitting to Eq. 36. Inset: Numerical estimates of $\varepsilon_1$ as a function of $\Delta$ (open circles) and the exact result, Eq. 37 (solid curve).

The bulk energy $\varepsilon_0(m)$ can be obtained exactly by solving Bethe ansatz integral equations, while the boundary energy $\varepsilon_1(m)$ is related to Eq. 26. Here, we fit the numerical data to the formula, taking $\varepsilon_0$, $\varepsilon_1$, and $\varepsilon_2$ as free parameters. The data of $E(L,m)$ at $\Delta = 0.8$ are shown in Fig. 1 for several values of $m$. We have found that the fitting works pretty well for all $\Delta$s and $m$s calculated. In fact, the estimated values of $\varepsilon_0$ obtained from the fitting are in excellent agreement with the exact values calculated from the Bethe ansatz equations (see Fig. 2). The bulk energy $\varepsilon_0(m)$ has smooth quadratic dependence on $m$ since the irrelevant operator $\cos(2\pi/R)$ yields only subleading contributions to the bulk quantity.

According to Eq. 26 and the relation between the bulk magnetization and the external field ($m = \chi_0 h/L$), the boundary energy $\varepsilon_1(m)$ should depend on $m$ as

$$\varepsilon_1(m) = \varepsilon_1(0) - h_1(2\pi m)^{\frac{\eta}{\eta - 1}} - \frac{(2\pi m)^2}{2\chi_2}$$

for small $m$, where $\chi_2$ is a constant and the exact form of $h_1$ is

$$h_1 = \frac{\lambda \Gamma(3 - \frac{2}{\eta}) \sin[\pi(\frac{1}{\eta} - 1)]}{2(\frac{1}{\eta} - 1)(\frac{1}{\eta} - 1)}.$$  

Note that the boundary energy of the open spin chains should be twice that of the semi-infinite wire that we have considered in the analytic calculation. To estimate the coefficient $h_1$ numerically, we fit the data of $\varepsilon_1(m)$ to Eq. 37, taking $\varepsilon_1(0)$, $h_1$, and $\chi_2$ as free parameters. We show the $m$ dependence of $\varepsilon_1(m)$ and the fitting curves in Fig. 3. Clearly, the plot of $\varepsilon_1(m)$ versus $(2\pi m)^2$ shows large deviation from linear dependence on $(2\pi m)^2$, confirming the existence of the leading power-law term with the exponent $2/\eta - 1$, which emerges from the irrelevant operator $\lambda \cos(2\phi/R)$. The values of $h_1$ estimated from the fitting procedure are also shown in Fig. 3. We see that the numerical estimates agree extremely well with the analytic result 37. This agreement can be regarded as a numerical proof of our analytic result, Eq. 26.

In summary, we have obtained the exact leading boundary contributions to the specific heat and the susceptibility using the low-energy effective theory for the spin-1/2 XXZ model. Our method can be easily extended to other 1D systems (e.g., the extended Hubbard model and spin ladders in high magnetic fields) as long as their low-energy effective theory is given by Eq. 3, which contains nonuniversal constants $\varepsilon$ and $\lambda$ to be determined with some other method, however. Our formulas 32, 33, and 34 for the spin isotropic case ($\Delta = 1$) are universal, in the sense that if we make any moderate deformation of the isotropic antiferromagnetic Heisenberg model that respects the SU(2) and translational symmetry and that does not generate a spin gap, then these formulas apply to some values of $T_0$ and $h_0$, except for cases where the coupling $\lambda$ is fine tuned to vanish. This implies that, for example, the 1D (extended) Hubbard model and other systems of interacting electrons with the spin SU(2) symmetry should universally exhibit the boundary contributions 32, 33, and 34.

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