Statistical Physics of Quantum Systems — novel orders and dynamics —
J. Phys. Soc. Jpn. Vol. 74 (2005) Suppl. pp. 36–41
©2005 The Physical Society of Japan

Boundary Critical Phenomena in the Heisenberg Spin-1/2 Chain with Open Ends

Satoshi FUJIMOTO[1]* and Sebastian EGGERT[2,3]

[1] *Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
[2] *Department of Physics, The University of Kaiserslautern, 67663 Kaiserslautern, Germany*
[3] *Institute of Theoretical Physics, Chalmers University of Technology, S-41296 Göteborg, Sweden*

(Received October 01, 2004)

We present a brief review on the recent theoretical developement about boundary effects in one-dimensional quantum spin systems focusing on the application of boundary conformal field theory. We discuss about low-temperature behaviors of the boundary contributions of the spin susceptibility and the specific heat coefficient. The anomalous behaviors at boundaries are deeply related with finite-temperature corrections of the boundary entropy or the ground state degeneracy, which yields a highly sensitive response of spin excitations in the vicinity of open boundaries.

KEYWORDS: Heisenberg spin chains, boundary critical phenomena, boundary conformal field theory

1. Introduction

In the last decade, effects of open boundaries in quantum one-dimensional (1D) spin systems have been extensively studied in connection with impurity problems.[1–3] Open boundaries in 1D quantum systems are introduced, for example, by a non-magnetic impurity which cuts a 1D system into two semi-infinite chains. Elaborate theoretical methods such as Bethe ansatz exact solutions and boundary conformal field theory, as well as various numerical simulations have been successfully applied to the investigation of boundary effects, and elucidated a lot of interesting features of boundary critical phenomena associated with open ends.[3–20] In the present paper, we review the recent developement on this issue with particular emphasis on the boundary conformal field thery approach.

One important ingredient of boundary critical phenomena is the emergence of boundary critical exponents corresponding to boundary operators. This aspect has been extensively studied so far.[4,8–10,21,22] Another interesting feature is related to the existence of a zero-temperature entropy $S_{\mathrm{B}} = \ln g$, where g is the ground state degeneracy. g is expressed as $\langle 0|B\rangle$ in terms of the ground state $|0\rangle$ and the boundary state $|B\rangle$. At critical points, g is universal, and constant, characterizing the universality class of boundary critical phenomena.[23] However when a system is off-critical at finite temperatures, S_{B} may vary with temperatures. This happens in the case that the system deviates from the low-energy fixed point due to bulk irrelevant interactions.[23,24] These interactions together with the redundant degrees of freedom may give rise to a non-trivial behavior of boundary parts of thermodynamic quantities such as the impurity spin susceptibility and the impurity specific heat coefficient. It should be noted that these quantities exhibit singular behaviors even at zero temperature as a function of the magnetic field h. For example, according to the Bethe ansatz solutions at zero temperature for the spin-1/2 Heisenberg chains, the SUSY t-J model, and the Hubbard model, the boundary susceptibility behaves like, $\chi_{\mathrm{B}} \sim 1/[4h\{\ln(h)\}^2]$ in the case with spin rotational symmetry.[11–14] This divergent behavior for a small magnetic field stems from the surface energy perturbed by leading irrelevant interactions. It was suggested in ref.[14] that at finite temperatures, in addition to the surface energy, the boundary entropy perturbed by bulk irrelevant interactions also yields a singular contribution as a function of temperature. In the case that the low-energy fixed point is the Tomonaga-Luttinger liquid, namely, the Gaussian model with the central charge $c = 1$, the boundary entropy is given by $S_{\mathrm{B}} = \ln(1/\sqrt{2R})$ for the Dirichlet boundary condition, where R is the radius parameter of the Gaussian model. Thus at finite temperatures or with a magnetic field, the presence of irrelevant interactions gives corrections to R and S_{B}, leading the singular temperature or field dependence of boundary quantities. This phenomenon is the main topic of the present paper.

The organization of this paper is as follows. In the sections 2 and 3, we give a pedagogic review on the low-energy effective field theory for the spin-1/2 XXZ chain, and some results of boundary conformal field theory relevant to our argument. In the section 4, a brief historical overview on this issue is presented. The recent results for the low-temperature dependence of the spin susceptibility and the specific heat coefficient caused by boundary effects are explained in the sections 5 and 6. The implication for experiments and a summary are given in the last section.

2. Low-energy effective field theory

Before discussing boundary effects, we would like to summarize the results of the bulk effective low-energy theory for quantum Heisenberg spin chains with $s = 1/2$ which is the basis of our analysis. The Hamiltonian for the spin-1/2 antiferromagnetic Heisenberg spin chains is given by

$$H_{XXZ} = J \sum [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z]. \qquad (1)$$

In the massless region, $0 \leq \Delta \leq 1$, the low energy fixed point of (1) is the Tomonaga-Luttinger liquid, which be-

*E-mail address: fuji@scphys.kyoto-u.ac.jp

longs to the universality class of the Gaussian theory with the central charge $c = 1$. In this case, the low energy effective Hamiltonian with the exact leading irrelevant interactions has been obtained by Lukyanov.[25] In the case of $0 \leq \Delta \leq 1/2$ ($K \geq 3/2$), the low-temperature anomalous behaviors at boundaries do not appear, as is easily seen from the dimensional analysis. Thus we will not consider this case.

For $1/2 < \Delta < 1$, the effective Hamiltonian is written as,

$$H = H_0 + H_{int}, \tag{2}$$

$$H_0 = \int_0^L \frac{dx}{2\pi}[(\partial_x\phi)^2 + (\partial_x\theta)^2], \tag{3}$$

$$H_{int} = a^{2K-2}\lambda\int_0^L \frac{dx}{2\pi}\cos(\sqrt{8K}\phi). \tag{4}$$

Here L is the linear system size, and the constants K, a, and λ are parametrized as, $K = [1 - \cos^{-1}(\Delta)/\pi]^{-1}$, $a = 2(K-1)/[JK\sin(\pi/K)]$, and

$$\lambda = \frac{4\Gamma(K)}{\Gamma(1-K)}\left[\frac{\Gamma(1+1/(2K-2))}{2\sqrt{\pi}\Gamma(1+K/(2K-2))}\right]^{2K-2}. \tag{5}$$

For this choice of the lattice constant a, the velocity of spinons is scaled to be unity. The boson fields $\phi(x)$ and $\theta(x)$ satisfy the canonical conjugate relation, $[\phi(x), \partial_x\theta(x')] = i\pi\delta(x - x')$. It is convenient to decompose $\phi(x)$ and $\theta(x)$ into the left-moving and right-moving parts; $\phi(x) = \phi_L(x) + \phi_R(x)$, $\theta(x) = \theta_L(x) - \theta_R(x)$. The mode expansions of these fields are given by

$$\phi_L(x,t) = \frac{q}{2} + \frac{\pi}{L}\left(\frac{P}{2} + \frac{\hat{w}}{\sqrt{2K}}\right)(t+x) + \frac{i}{2}\sum_{n\neq 0}\frac{1}{n}\alpha_n e^{-i\frac{2\pi n}{L}(t+x)} \tag{6}$$

$$\phi_R(x,t) = \frac{\bar{q}}{2} + \frac{\pi}{L}\left(\frac{P}{2} - \frac{\hat{w}}{\sqrt{2K}}\right)(t-x) + \frac{i}{2}\sum_{n\neq 0}\frac{1}{n}\bar{\alpha}_n e^{-i\frac{2\pi n}{L}(t-x)}. \tag{7}$$

The canonical conjugate relation leads the following commutation relations,

$$[\alpha_n, \alpha_m] = [\bar{\alpha}_n, \bar{\alpha}_m] = n\delta_{n+m,0}, \quad [\alpha_n, \bar{\alpha}_m] = 0, \tag{8}$$

$$[q, P] = i, \quad [\bar{q}, P] = i, \quad [P, \hat{w}] = 0, \tag{9}$$

$$[\bar{q}, q] = i\pi, \quad [q, \hat{w}] = i\frac{\sqrt{2K}}{2}, \quad [\bar{q}, \hat{w}] = -i\frac{\sqrt{2K}}{2}. \tag{10}$$

The last three commutation relations are required to ensure the anti-commutation relations of fermions related to spin operators via the Jordan-Wigner transformation. The eigenvalue of $\hat{w}$ is an integer w corresponding to the winding number of the phase field ϕ.

For the $c = 1$ Gaussian theory, as will be shown later, boundary states are constructed from the highest weight state (the primary state) of the U(1) Kac-Moody algebra $|v, w\rangle$ which is the eigenstate of the zero mode of α_n, $\bar{\alpha}_n$ defined as,

$$\alpha_0 = \frac{P}{2} + \frac{w}{\sqrt{2K}}, \qquad \bar{\alpha}_0 = \frac{P}{2} - \frac{w}{\sqrt{2K}}. \tag{11}$$

The state $|v, w\rangle$ specified by integers v and w satisfies the eigenvalue equations,

$$\alpha_0|v,w\rangle = \left(\frac{\sqrt{2K}v}{2} + \frac{w}{\sqrt{2K}}\right)|v,w\rangle, \tag{12}$$

$$\bar{\alpha}_0|v,w\rangle = \left(\frac{\sqrt{2K}v}{2} - \frac{w}{\sqrt{2K}}\right)|v,w\rangle. \tag{13}$$

Thus, $|v, w\rangle$ is an energy eigenstate of the Gaussian model;

$$H_0|v,w\rangle = \frac{2\pi}{L}(\Delta^+_{vw} + \Delta^-_{vw} - \frac{1}{12})|v,w\rangle, \tag{14}$$

$$\Delta^\pm_{vw} = \frac{1}{2}\left(\frac{\sqrt{2K}v}{2} \pm \frac{w}{\sqrt{2K}}\right)^2. \tag{15}$$

Using the finite size scaling argument, we can read off the conformal dimension $\Delta^+_{vw} + \Delta^-_{vw}$ for the primary field,

$$\exp(iv\sqrt{2K}\phi(x,t) + iw\sqrt{2/K}\theta(x,t)). \tag{16}$$

This primary field corresponds to the primary state $|v, w\rangle$.

At the isotropic point $\Delta = 1$ ($K = 1$), the effective low-energy theory is described by the level $k = 1$ SU(2) Wess-Zumino-Witten model with a marginally irrelevant interaction:

$$H = H_{WZW} + H_m, \tag{17}$$

$$H_m = -g\int_0^L \frac{dx}{2\pi}\sum_{a=1}^{3} J^a(x)\bar{J}^a(x). \tag{18}$$

Here H_{WZW} is the Hamiltonian of the level $k = 1$ SU(2) Wess-Zumino-Witten model, and $J^a(x)$ ($\bar{J}^a(x)$) is the left (right) moving current of the level $k = 1$ SU(2) Kac-Moody algebra. The running coupling constant g depends on temperature T and an external magnetic field h through the scaling equation,[25]

$$g^{-1} + \frac{1}{2}\ln(g) = -\mathrm{Re}[\psi(1 + \frac{ih}{2\pi T})] + \ln(\sqrt{2\pi}e^{1/4}J/T), \tag{19}$$

with $\psi(x)$ the di-gamma function.

Generally, in 1D quantum systems with boundaries, there may be boundary interactions in addition to bulk interactions. However, as was pointed out in ref.,[16] in the absence of symmetry-breaking external fields at boundaries, irrelevant boundary interactions do not give singular contributions to boundary quantities, and are negligible in the following argument.

3. Boundary conformal field theory for the $c = 1$ Gaussian model

Here we briefly review some results of boundary conformal field theory which will be used in the following calculations.

In general, for two-dimensional (or quantum 1D) critical field theories, any system is invariant under the conformal transformation which is generated by the holomorophic and anti-holomorophic parts of the stress tensor $T(z)$, $\bar{T}(\bar{z})$. For a cylinder with perimeter $1/T$, the mode expansions are expressed as,

$$T(x+\mathrm{i}y) = (2\pi T)^2 \sum_n e^{2\pi T(x+\mathrm{i}y)}(L_n - \frac{c}{24}\delta_{n0}), \quad (20)$$

$$\bar{T}(x-\mathrm{i}y) = (2\pi T)^2 \sum_n e^{2\pi T(x-\mathrm{i}y)}(\bar{L}_n - \frac{c}{24}\delta_{n0}), \quad (21)$$

where L_n and $\bar{L}_n$ are the Virasoro generators. For the Gaussian model with $c=1$, the Virasoro generators have the free boson representation,

$$L_0 = \frac{\alpha_0^2}{2} + \sum_{n=1}^{\infty} \alpha_{-n}\alpha_n, \quad \bar{L}_0 = \frac{\bar{\alpha}_0^2}{2} + \sum_{n=1}^{\infty} \bar{\alpha}_{-n}\bar{\alpha}_n, \quad (22)$$

and,

$$L_n = \frac{1}{2}\sum_m :\alpha_{n-m}\alpha_m:, \quad \bar{L}_n = \frac{1}{2}\sum_m :\bar{\alpha}_{n-m}\bar{\alpha}_m: \quad (23)$$

for $n \neq 0$.

For two-dimensional systems with a boundary at $x=0$ ($z = x+\mathrm{i}y$), a conformally invariant boundary condition is imposed by demanding that $T(z) = \bar{T}(\bar{z})$ on the boundary.[22] For the Gaussian model with $c=1$, we see from eqs.(20)-(23) that this condition is fullfilled under the following stronger constraint on the boundary state,[26–28]

$$(\alpha_n \pm \bar{\alpha}_{-n})|B\rangle = 0, \quad (24)$$

where the plus (minus) sign corresponds to the Neumann (Dirichlet) boundary condition. The solution for (24) is expressed in terms of the Ishibashi state.[21,29] For the Dirichlet condition, it is given by,[26–28]

$$|D\rangle = \left(\frac{K}{2}\right)^{\frac{1}{4}} \sum_{v=-\infty}^{\infty} e^{-i\sqrt{2K}v\phi_0} \exp\left(-\sum_{n=1}^{\infty}\frac{\alpha_{-n}\bar{\alpha}_{-n}}{n}\right)|v,0\rangle. \quad (25)$$

Note that the prefactor $(K/2)^{1/4}$ is the boundary degeneracy at zero temperature, which is related to the boundary entropy $S_{\mathrm{B}} = \ln(K/2)^{1/4}$. S_{B} is non-zero when non-trivial bulk correlations exist; i.e. $K \neq 2$. The constant ϕ_0 is the eigenvalue of the boson field ϕ at the boundary. The boundary state for the Neumann condition is,[26–28]

$$|N\rangle = \left(\frac{1}{2K}\right)^{\frac{1}{4}} \sum_{w=-\infty}^{\infty} e^{-i\sqrt{2/K}w\theta_0} \exp\left(\sum_{n=1}^{\infty}\frac{\alpha_{-n}\bar{\alpha}_{-n}}{n}\right)|0,w\rangle, \quad (26)$$

where θ_0 is the boundary value of the dual field, $\theta(x)$. The prefactor $(1/2K)^{1/4}$ is also the boundary degeneracy for this boundary condition.

4. Boundary effects in the $s = 1/2$ spin chains — A brief overview

As mentioned before, non-magnetic impurities in quantum spin chains can be effectively regarded as free open boundaries provided that the interaction between two open ends separated by a non-magnetic impurity is negligible. In such a case, non-trivial boundary effects emerge in the thermodynamic limit $N \gg J/T$, where N is the system size. In contrast, in the oppsite limit $T/J \ll 1/N$ the behavior is trivially described by the ground state, which is a singlet for even N with exponentially small susceptibility as $T \to 0$ and a doublet for odd N with a Curie law behavior. In the present paper, we mainly consider the thermodynamic limit $1/N \ll T/J \ll 1$, which highlights intriguing boundary correlation effects.

The application of the boundary conformal field theory to impurity issues in the $s=1/2$ quantum spin chains was first considered by Eggert and Affleck a decade ago.[3] As was discussed in that paper, the free open boundary condition at $x=0$ for spin chains is that the magnetization current at the boundary $J^z(x=0,t)$ must vanish, though the boundary magnetization at $x=0$ is not fixed to a particular value. In terms of the low-energy effective field theory, this condition is expressed as $\phi_L(x=0,t) + \phi_R(x=0,t) = 0$, which allows us to define $\phi_R(x,t)$ as the analytic continuation of $\phi_L(x,t)$ to the negaitive axis: $\phi_R(x,t) = -\phi_L(-x,t)$. We can easily see that this relation actually fulfill the above-mentioned requirement; i.e. $S^z(x=0,t) \propto \partial_x\phi_L(x,t)|_{x=0}$, and $J^z(x=0,t) = \partial_t\phi_L(0,t) + \partial_t\phi_R(0,t) = 0$. Then, the effective field theory is expressed only in terms of the left-moving part ϕ_L.

Boundary critical phenomena appear in the long-time behavior of boundary correlation functions. At the zero-temperature fixed point described by the free boson, the above boundary condition does not affect the uniform part of the spin-spin correlation functions, but change the staggered part drastically. Neglecting the irrelevant interaction (4) or (18), Eggert and Affleck obtained the impurity part of the spin structure factor which behaves $S_{\mathrm{imp}}(k \sim \pi) \propto v/T$ at low temperatures, reflecting enhanced antiferromagnetic correlation in the vicinity of the open boundaries. No singular temperature behavior of the impurity uniform suscepetibility was predicted however.

On the other hand, the Bethe ansatz exact solution at $T=0$ predicts that the boundary uniform susceptibiltiy behaves $\chi_{\mathrm{B}} = 1/[4h(\ln(h))^2]$ for small magnetic field, implying the singular temperature dependence of the uniform part, in contrast to the above field theoretical result. Since boundary irrelevant interactions merely give small corrections to the spin susceptibility, the origin of the singular behavior may be attributed to bulk interactions ignored in the analysis of ref.[3] The importance of the bulk irrelevant interactions for boundary critical phenomena was also discussed before by Affleck and Qin,[15] and Brunel et al.[16] in connection with logarithmic corrections to the nuclear relaxation rate $1/T_1$ at the boundary. For the isotropic spin chain, it is given by, $1/T_1 \propto T[\ln(T_0/T)]^2$, which makes a sharp contrast to the behavior of the system without boundaries, $1/T_1 \propto [\ln(T_0/T)]^{1/2}$. This result is due to the interplay between the existence of the boundary entropy and the surface energy, and the bulk marginally irrelevant interaction.

As will be explained in the next sections, a similar effect crucially controls the low temperature behaviors of the boundary spin susceptibility and the boundary specific heat coefficient.

5. Boundary conformal perturbation theory for spin-1/2 chains

In this section, using the results from sections 2 and 3, we show that boundary quantities exhibit a singular temperature dependence, which stems from the boundary entropy and the surface energy perturbed by bulk irrelevant interactions. For this purpose, following the idea of Cardy and Lewellen,[21] we consider the geometry of a semi-infinite cylinder with perimeter $1/T$. Interchanging space and time coordinates, we define the phase field on this geometry as,

$$\phi^c(x,t) = Q + \pi TPx + 2\pi T\frac{wt}{\sqrt{2K}} + \frac{i}{2}\sum_{n\neq 0}\frac{1}{n}(\alpha_n e^{-i2\pi Tn(x+t)} + \bar{\alpha}_n e^{-i2\pi Tn(x-t)}). \quad (27)$$

Then, the Hamiltonian on the semi-infinite cylinder is written as,

$$H^c = H_0^c + H_{int}^c, \quad (28)$$

$$H_0^c = \int_0^{1/T}\frac{dt}{2\pi}[(\partial_t\phi^c)^2 + (\partial_x\phi^c)^2], \quad (29)$$

$$H_{int}^c = a^{2K-2}\lambda\int_0^{1/T}\frac{dt}{2\pi}\cos(\sqrt{8K}\phi^c). \quad (30)$$

We express the partition function by using the transfer matrix $\exp(-LH^c)$ and the boundary state $|B\rangle$. The lowest order terms of the free energy are given by,

$$F = -\frac{aT}{L}\ln\langle 0|e^{-LH_0^c}|B\rangle + \frac{aT}{L}\int_0^L dx\frac{\langle 0|\exp(-LH_0^c)\exp(xH_0^c)H_{int}^c\exp(-xH_0^c)|B\rangle}{\langle 0|\exp(-LH_0^c)|B\rangle} + \cdots, \quad (31)$$

where $|0\rangle$ is the ground state of H_0^c. The first term of the right-hand side of (31) is the free energy of the $c=1$ Gaussian model. The second term, which is denoted by $\delta F_{\rm B}$ in the following, is the $1/L$ correction that emerges as a result of boundary effects. $\delta F_{\rm B}$ is expressed in terms of the one-point function of the primary field $\Phi(x,\tau)\equiv\exp(i\sqrt{8K}\phi(x,\tau))$ which has the conformal dimension $2K$,

$$\delta F_{\rm B} = \frac{a^{2K-1}T\lambda}{2\pi L}\int_0^L dx\int_0^{1/T}d\tau(\langle\Phi(x,\tau)\rangle_B + h.c.)/2. \quad (32)$$

At this stage, the effect of a magnetic field is incorporated by shifting the boson field $\phi^c(x)$ to $\tilde{\phi}^c(x) = \phi^c(x) - \sqrt{K/2}hx$. Following Cardy and Lewellen,[21] we apply the conformal transformation from the cylinder $z = x + i\tau$ to the semi-infinite plane ${\rm Im}z' > 0$: $z = (2\pi T)^{-1}\ln[(1-iz')/(1+iz')]$. Then, the boundary term is rewritten as,

$$\delta F_{\rm B} = \frac{a^{2K-1}T\lambda}{2\pi L}\int_0^L dx\int_0^{1/T}d\tau\frac{(\pi T)^{2K}}{|1+z'^2|^{2K}} \times(\langle\Phi'(z',\bar{z}')\rangle_B + h.c.)/2. \quad (33)$$

For the semi-infinite plane, the average of the local operator close to a boundary is computed by the standard method,

$$\langle\Phi'(z',\bar{z}')\rangle_B = \langle\Phi'_L(z')\Phi'_R(\bar{z}')\rangle_B \sim \langle\Phi'_L(z')\Phi'_L(\bar{z}')\rangle_B \sim \frac{A_\Phi^B}{(2{\rm Im}z')^{2K}}, \quad (34)$$

with $\Phi'_{L(R)}$ the (anti-)holomorphic part of $\Phi'(z',\bar{z}')$, and A_Φ^B the coefficient of the operator product expansion. Regulating the ultra-violet divergence of eq. (34) via point-splitting procedure, and transforming back to the z-coordinate, we have

$$\delta F_{\rm B} = -\frac{A_\Phi^B\lambda(\pi aT)^{2K}}{2\pi aL}\int_a^L dx\frac{\cos(2Khx)}{[\sinh(2\pi Tx)]^{2K}}. \quad (35)$$

By using the point-splitting procedure, we have discarded a non-universal divergent term which is not important for the low-energy properties. The constant A_Φ^B is obtained by considering the long distance behavior of $\langle\Phi(x,\tau)\rangle_B$ for large x,

$$\langle\Phi(x,\tau)\rangle_B \sim \frac{\langle 0|\Phi|\Phi\rangle\langle\Phi|B\rangle}{\langle 0|B\rangle}\exp(-4\pi TKx). \quad (36)$$

Here $|\Phi\rangle$ is the primary state corresponding to the conformal field $\Phi(x,\tau)$. Comparing eqs. (33), (34), and (36), and using $\langle 0|\Phi|\Phi\rangle = (2\pi T)^{2K}$, we end up with,

$$A_\Phi^B = \frac{\langle\Phi|B\rangle}{\langle 0|B\rangle}. \quad (37)$$

The matrix element between $|0\rangle$ and $|B\rangle$ that appears in (37) can be computed by using (25) and (26). We see from eqs. (15) and (16) that $|\Phi\rangle$ is the primary state $|2,0\rangle$. $\langle\Phi|B\rangle$ is non-vanishing, only if $|B\rangle$ contains $|2,0\rangle$. The Neumann boundary state (26) does not satisfy this condition, leading $\langle\Phi|N\rangle = 0$. On the other hand, $\langle\Phi|D\rangle$ gives a finite contribution. The averaged value of the phase ϕ_0 at the boundary is set to $\phi_0 = 0$, which is consistent with the free open boundary condition for the boundary magnetization. Then, from eq. (25), we have $\langle 2,0|D\rangle/\langle 0|D\rangle = 1$.

The Dirichlet boundary condition corresponds to the absence of the spin current leaking from the open ends. This is easily seen as follows. From eq. (27), the spin current operator at the boundary $x=0$ obeys,

$$J_s \equiv i\partial_\tau\phi^c(x=0,\tau) = i\pi T\sum_{n=-\infty}^{\infty}(\alpha_n - \bar{\alpha}_{-n})e^{-i2\pi Tn\tau}. \quad (38)$$

The boundary condition (24) leads $J_s|B\rangle = 0$ for the Dirichlet condition. We would like to stress that since the time and space coordinates are interchanged in eq. (27), the canonical conjugate field of ϕ^c is not $\partial_\tau\phi^c$, but $\partial_x\phi^c$. Thus, we can fix the boundary average values of $\phi^c(x=0)$ and $\partial_\tau\phi^c(x=0)$ simultaneously for the Dirichlet condition. This implies that the average value of the local magnetization at the boundary $\sim\partial_x\phi^c(x=0)$ is not fixed to a particular value, fulfilling the free open boundary condition with which we are concerned.

5.1 *Field theoretical results for boundary quantities*

5.1.1 *The anisotropic case* $1/2 < \Delta < 1$

The corrections to the boundary free energy caused by the irrelevant interaction is computed from eqs. (35) as,

$$\delta F_{\mathrm{B}} = -\frac{\lambda}{4\pi L}(2\pi aT)^{2K-1}\mathrm{Re}[B(K+i\frac{Kh}{2\pi T}, 1-2K)], \tag{39}$$

where $B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$. In the case that the system has two open boundaries, the boundary term of the free energy is given by twice F_{B}.

Usng eq. (39), we calculate the leading temperature dependence of the boundary spin susceptibility contributed from two open ends,

$$\chi_{\mathrm{B}} = \frac{\lambda a K^2}{2\pi}B(K,1-2K)[\pi^2 - 2\psi'(K)](2\pi aT)^{2K-3}, \tag{40}$$

with $\psi'(x) = d\psi(x)/dx$. Note that for $1 < K < 3/2$ ($1/2 < \Delta < 1$), the boundary spin susceptibility χ_{B} shows a divergent behavior $\sim 1/T^{3-2K}$, as temperature decreases. This anomalous temperature dependence is also observed in the boundary part of the specific heat coefficient given by,

$$\frac{C_{\mathrm{B}}}{T} = 2\pi a\lambda(2K-1)(2K-2)B(K,1-2K)(2\pi aT)^{2K-3}. \tag{41}$$

We would like to stress that in the formulas (40) and (41) there is no free parameter, and the prefactors are exactly obtained. The divergent behaviors can physically be understood as follows. In contrast to the bulk Heisenberg chains in which the ground state is a spin singlet state, spin singlet formation in the vicinity of boundaries is strongly disturbed by thermal fluctuation, because of the enhanced correlation at the boundaries which stems from the ground state degeneracy. It should be emphasized again that the singular behaviors are not due to the presence of boundary operators, but interpreted as a consequence of finite-temperature corrections of the surface energy and the boundary entropy $\ln\langle 0|B\rangle$ caused by bulk irrelevant interactions.

At zero temperature with a finite magnetic field, a similar singular behavior appears in the field dependence of the boundary spin susceptibility given by,

$$\chi_{\mathrm{B}}(T=0) = \frac{\lambda(aK)^{2K-1}}{2\pi a}\sin(\pi K)\Gamma(3-2K)h^{2K-3}. \tag{42}$$

We have checked that this result coincides with that obtained from the Bethe ansatz exact solution.

5.1.2 *The isotropic case* $\Delta = 1$

Now let us consider the isotropic case $K = 1$. The free energy correction (39) possesses poles for $K = 1$. To deal with these singularities, we follow the procedure considered by Lukyanov for bulk spin systems.[25)] We rewrite H_{int} in terms of the SU(2) current operators,

$$H_{int} = \int \frac{dx}{2\pi}[g_{\parallel}J_0\bar{J}_0 + \frac{g_{\perp}}{2}(J_+\bar{J}_- + J_-\bar{J}_+)]. \tag{43}$$

The exact expressions for the running coupling constants $g_{\parallel}$ and $g_{\perp}$ are given in ref.[25,30)] On the other hand, for the value of K close to 1, eq. (39) can be expanded in power series of $1 - 1/K$. Comparing the expansion of eq. (39) with the expression for $g_{\parallel}$ and $g_{\perp}$, we can write the free energy correction (39) as a power series expansion in terms of $g_{\parallel}$ and $g_{\perp}$. Then, taking the limit $K \to 1$ and $g_{\parallel}, g_{\perp} \to g$, we end up with,

$$2\delta F_{\mathrm{B}} = -\frac{Tg}{2N} - \frac{h^2}{24NT}(g+g^2) + ... \tag{44}$$

for $h \ll T$. The running coupling constant g obeys eq. (19). From eq. (44), we obtain the leading term of the boundary spin susceptibility and the specific heat coefficient,

$$\chi_{\mathrm{B}} = \frac{1}{12T\ln(\alpha/T)}\left(1 - \frac{\ln\ln(\alpha/T)}{2\ln(\alpha/T)} + ...\right), \tag{45}$$

$$\frac{C_{\mathrm{B}}}{T} = \frac{1}{2T(\ln(\alpha/T))^2}\left(1 - \frac{\ln\ln(\alpha/T)}{\ln(\alpha/T)} + ...\right), \tag{46}$$

where $\alpha = \sqrt{\pi/2}\exp(1/4+\gamma)$ with γ the Euler constant. At zero temperature, the boundary spin susceptibility for a small magnetic field is also derived from the opposite limit $h \gg T$ of eq. (39), The result coincides completely with that obtained from the Bethe ansatz exact solutions.[11–14)]

In an independent work, Furusaki and Hikihara have also derived the results (40), (45), (41), and (46) using conventional bosonization methods.[20)]

6. Comparison with numerical results

In this section, we present a comparison between the field theoretical results obtained in the previous sections and numerical calculations based upon the density matrix renormalization group for transfer matrices (TMRG) applied to impurity problems.[17)] This method is suitable for the calculation of local expectation values and the impurity free energy in the thermodynamic limit $N \to \infty$. When we compute the impurity susceptibility, we need to take the second derivative of the impurity free energy and therefore subtract two large numbers, which turns out to be inaccurate for very low temperatures. For the lowest temperatures ($T < 0.1J$) we have instead summed over the excess local responses in a range around the open ends, which yielded more accurate results. This method agrees with taking the second derivative for higher T and should also be a good approximation for $T < 0.1J$. As shown in Fig. 1 (upper panel), the numerical results obtained by this method agree well with the field theoretical results without any adjustable parameters.

7. Discussion and Summary

The Curie-like temperature dependence with logarithmic corrections of the boundary spin susceptibility (45) may be relevant to experimental observations. According to experimental measurements of the spin susceptibility for the Heisenberg spin chains such as Sr_2CuO_3, a Curie-like behavior at low temperature region is always observed, but has been regarded as an extrinsic impurity effect.[32)] Since the Curie contribution is strongly reduced by careful annealing,[32,33)] this Curie tail cannot be due to magnetic impurities in the sample. For extremely low temperatures $T/J \ll 1/N$ such a Curie

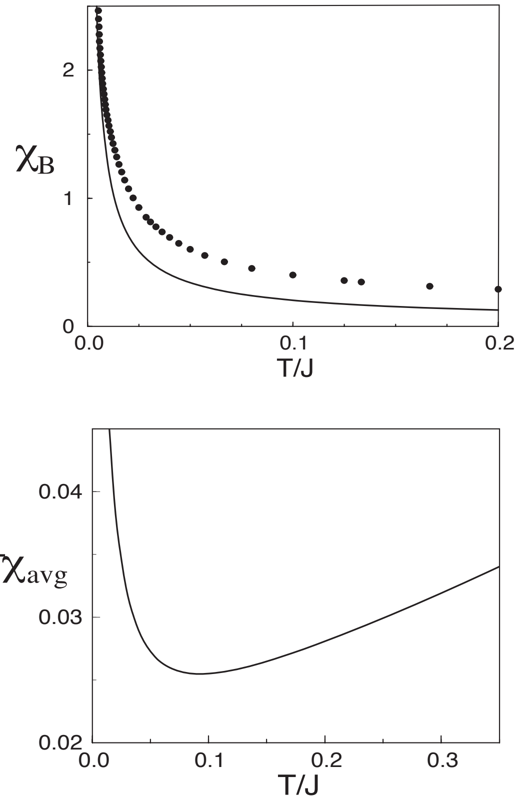

Fig. 1. Upper panel: the boundary susceptibility χ_B as a function of T obtained from the TMRG calculations (black points). The solid line is the plot of the field theoretical result eq. (45). Lower panel: approximate temperature dependence of the average Curie constant per impurity for an impurity density of $\rho = 0.1\%$

behavior can be explained by the trivial size effect of finite chains with odd N that have locked into their doublet ground state.[18] For higher temperatures, however, a Curie-like behavior may be attributed to non-trivial boundary effects given by eq. (45). The crossover between these two different regions occurs when the temperature becomes comparable to the finite size energy gap $T \sim \pi v/N$. For a carefully annealed sample of Sr_2CuO_3 with $\rho \sim 0.013\%$[32] the ground state contribution is only significant for $T < 0.001J \sim 2K$. Thus the averaged Curie constant varies with temperatures showing a minumim around the crossover temperature. The approximate behavior of the averaged Curie constant for the impurity susceptibility $T\chi_{\rm avg}$ is shown in Fig. 1 (lower panel) for $\rho = 0.1\%$ by averaging over all chain lengths and assuming a sharp crossover from ground state to thermodynamic behavior.

In summary, we have given a short review on boundary critical phenomena related to 1D quantum spin chains with open ends with emphasis on the application of the boundary conformal field theory, and the role of the zero-temperature boundary entropy.

Acknowledgement

We would like to thank I. Affleck, F.H.L. Essler, A. Furusaki, and N. Kawakami for valuable discussions. This work was partly supported by a Grant-in-Aid from the Ministry of Education, Science, Sports and Culture, Japan.

1) M. Hagiwara, K. Katsumata, I. Affleck, B.I. Halperin, and J.P. Renard: Phys. Rev. Lett. **65** (1990) 3181; C.D. Batista, K. Hallberg, and A.A. Aligia: Phys. Rev. B **58** (1998) 9248.
2) S. Sachdev, C. Buragohain, and M. Vojta: Science **286** (1999) 2479; M. Vojta, C. Buragohain, and S. Sachdev: Phys. Rev. B **61** (2000) 15152; K.H. Höglund and A.W. Sandvik: Phys. Rev. Lett. **91** (2003) 077204.
3) S. Eggert and I. Affleck: Phys. Rev. B **46** (1992) 10866; Phys. Rev. Lett. **75** (1995) 934.
4) F.C. Alcaraz, M. N. Barber, M. T. Batchelor, R.J. Baxter, and G.R.W.Quispel: J. Phys. A **20** (1987) 6397.
5) M. Shiroishi and M. Wadati: J. Phys. Soc. Jpn. **66** (1997) 1.
6) R. Yue and T. Deguchi: J. Phys. A**30** (1997) 8129.
7) P. de Sa and A. M. Tsvelik: Phys. Rev. B **52** (1995) 3067.
8) G. Bedürftig and H. Frahm: J. Phys. A **30** (1997) 4139.
9) S. Fujimoto and N. Kawakami: Phys. Rev. B**54** (1996) 5784.
10) H. Asakawa and M. Suzuki: J. Phys.A **29** (1996) 225.
11) F.H.L. Essler: J. Phys. A **29** (1996) 6183.
12) H. Asakawa and M. Suzuki: J. Phys. A **29** (1996) 225; *ibid* **29** (1996) 7811.
13) H. Frahm and A. A. Zvyagin: J. Phys.: Condens. Matter **9** (1997) 9939.
14) S. Fujimoto: Phys. Rev. B **63** (2000) 024406.
15) I. Affleck and S. Qin: J. Phys. A **32** (1999) 7815.
16) V. Brunel, M. Bocquet, and Th. Jolicoeur: Phys. Rev. Lett. **83** (1999) 2821.
17) S. Rommer and S. Eggert: Phys. Rev. B **59** (1999) 6301; *ibid* **62** (2000) 4370.
18) S. Wessel and S. Haas: Phys. Rev. B **61** (2000) 15262.
19) S. Fujimoto and S. Eggert: Phys. Rev. Lett. **92** (2004) 037206.
20) A. Furusaki and T. Hikihara: Phys. Rev. B **69** (2004) 094429.
21) J. L. Cardy and D. C. Lewellen: Phys. Lett. B **259** (1991) 274.
22) J. L. Cardy: Nucl. Phys. B **324** (1989) 581.
23) I. Affleck and A. W. W. Ludwig: Phys. Rev. Lett. **67** (1991) 161.
24) Very recently, the renormalization flow of the boundary entropy is precisely discussed by D. Friedan and A. Konechny: Phys. Rev. Lett. **93** (2004) 030402.
25) S. Lukyanov: Nucl. Phys. B **522** (1998) 533.
26) C. G. Callan, C. Lovelace, and C. R. Nappi, and S. A. Yost: Nucl. Phys. B **293** (1987) 83.
27) C. G. Callan, I. R. Klebanov, A. W. W. Ludwig, and J. M. Maldacena: Nucl. Phys. B **422** (1994) 417.
28) M. Oshikawa and I. Affleck: Nucl. Phys. B **495** (1997) 533.
29) N. Ishibashi, Mod: Phys. Lett. A **4** (1989) 251.
30) Al.B. Zamolodchikov Int. J. Mod: Phys. A **10** (1995) 1125.
31) S. Eggert, unpublished.
32) N. Motoyama, H. Eisaki, and S. Uchida: Phys. Rev. Lett. **76** (1996) 3212.
33) T. Ami, M.K. Crawford, R.L. Harlow, Z.R. Wang, D.C. Johnston, Q. Huang, R.W. Erwin: Phys. Rev. B **51** (1995) 5994.