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Boundary susceptibilities of the Hubbard model in open chains

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Abstract. Boundary contributions to the magnetization and the electron density are evaluated analytically, near the half-filling and non-magnetic region. Boundary susceptibilities in the spin and the charge sectors are also calculated. The boundary magnetization approaches zero logarithmically as the magnetic field goes to zero. The boundary charge susceptibility diverges like the bulk compressibility when the filling goes to unity.

1. Introduction

Recently, one-dimensional strongly correlated systems with boundaries have attracted much attention. Some of these systems can be exactly solved by deriving Bethe-ansatz equations; for example, the XXZ model [1, 2], the interacting boson model [3], the interacting fermion model [4, 5] and the Hubbard model [6, 7]. Using the Bethe-ansatz equations, finite-size corrections of the ground-state energies have been calculated [5, 7, 8] to discuss critical phenomena in such systems with boundaries. Moreover, boundary contributions to physical quantities have also been evaluated in some exactly solvable models, for example, the XXZ model [9], the supersymmetric t–J model [10].

In the present study, we discuss the Hubbard model in open chains described by

$$\mathcal{H} = -\sum_{j=1}^{L-1}\sum_{\sigma=\pm}(c_{j\sigma}^{\dagger}c_{j+1\sigma} + c_{j+1\sigma}^{\dagger}c_{j\sigma}) + 4u\sum_{j=1}^{L} n_{j+}n_{j-} + \mu\sum_{j=1}^{L}(n_{j+}+n_{j-}) - \frac{h}{2}\sum_{j=1}^{L}(n_{j+}-n_{j-}) \tag{1.1}$$

with $n_{j\sigma} = c_{j\sigma}^{\dagger}c_{j\sigma}$ and $u > 0$. Here, the symbol $c_{j\sigma}$ denotes the annihilation operator of the electron with spin σ at site j.

We evaluate the boundary magnetization (m^{b}) and the boundary electron density (n^{b}) in the ground state, which are defined by

$$m^{\mathrm{b}} \equiv -\frac{\partial}{\partial h}(E_L^{\mathrm{open}} - E_L^{\mathrm{periodic}}) \qquad \text{for } L \gg 1 \tag{1.2}$$

$$n^{\mathrm{b}} \equiv \frac{\partial}{\partial \mu}(E_L^{\mathrm{open}} - E_L^{\mathrm{periodic}}) \qquad \text{for } L \gg 1. \tag{1.3}$$

Here, we describe the ground-state energy in the Hubbard chain with L sites under the open (or periodic) boundary condition by the symbol E_L^{open} (or E_L^{periodic}). We also define the boundary spin susceptibility and the boundary charge susceptibility, as follows,

$$\chi_{\mathrm{s}}^{\mathrm{b}} = \frac{\partial m^{\mathrm{b}}}{\partial h} \qquad \text{and} \qquad \chi_{\mathrm{c}}^{\mathrm{b}} = -\frac{\partial n^{\mathrm{b}}}{\partial \mu} \tag{1.4}$$

respectively.

As is well known, the bulk contributions to the magnetization (or spin susceptibility) [11, 12] and the electron density (or charge susceptibility) [13] have been discussed in detail, using the Lieb–Wu solution [14] which is given by the Bethe-ansatz equation of the Hubbard model with the periodic boundary condition. On the other hand, in the present study, we use the the Bethe-ansatz equation of the Hubbard model with the open boundary condition [6] to derive m^{b} and n^{b}, analytically. Our strategy is as follows.

Now, we remember that the following expressions

$$\frac{E_L^{\text{periodic}}}{L} = \frac{1}{2\pi}\int_{-k_0}^{+k_0} \mathrm{d}k\, \varepsilon_{\mathrm{c}}(k) + \mathrm{O}\left(\frac{1}{L^2}\right) \tag{1.5}$$

have already been obtained for the periodic-boundary case [15] and

$$\begin{aligned}\frac{E_L^{\text{open}}}{L} = {} & \frac{1}{2\pi}\int_{-k_0}^{+k_0} \mathrm{d}k\, \varepsilon_{\mathrm{c}}(k) + \frac{1}{L}\left(1 - \frac{\mu}{2} - \frac{h}{4}\right) + \frac{1}{2L}\int_{-k_0}^{+k_0} \mathrm{d}k\, \varepsilon_{\mathrm{c}}(k)\left(\frac{1}{\pi} - a_1(\sin k)\cos k\right) \\ & + \frac{1}{2L}\int_{-\lambda_0}^{+\lambda_0} \mathrm{d}\lambda\, \varepsilon_{\mathrm{s}}(\lambda) a_2(\lambda) + \mathrm{O}\left(\frac{1}{L^2}\right)\end{aligned} \tag{1.6}$$

for the open-boundary case [7] with

$$a_\nu(x) = \frac{1}{2\pi}\frac{2\nu u}{(\nu u)^2 + x^2}. \tag{1.7}$$

In both cases, the symbols $\varepsilon_{\mathrm{c}}(k)$ and $\varepsilon_{\mathrm{s}}(\lambda)$ denote the dressed energies [15, 7] in the charge and spin sectors, respectively, which are defined by

$$\varepsilon_{\mathrm{c}}(k) = \varepsilon_{\mathrm{c}}^{(0)}(k) + \int_{-\lambda_0}^{+\lambda_0} \mathrm{d}\lambda\, a_1(\sin k - \lambda)\varepsilon_{\mathrm{s}}(\lambda) \tag{1.8}$$

$$\varepsilon_{\mathrm{s}}(\lambda) = \varepsilon_{\mathrm{s}}^{(0)}(\lambda) + \int_{-k_0}^{+k_0} \mathrm{d}k\, \cos k a_1(\lambda - \sin k)\varepsilon_{\mathrm{c}}(k) - \int_{-\lambda_0}^{+\lambda_0} \mathrm{d}\lambda'\, a_2(\lambda - \lambda')\varepsilon_{\mathrm{s}}(\lambda') \tag{1.9}$$

with

$$\varepsilon_{\mathrm{c}}^{(0)}(k) = \mu - \frac{h}{2} - 2\cos k \qquad \varepsilon_{\mathrm{s}}^{(0)}(\lambda) = h. \tag{1.10}$$

Here, we determine the parameters k_0 and λ_0 by

$$\varepsilon_{\mathrm{c}}(k_0) = 0 \qquad \text{and} \qquad \varepsilon_{\mathrm{s}}(\lambda_0) = 0. \tag{1.11}$$

For example, $\lambda_0 = \infty$ for $h = 0$, or $k_0 = \pi$ for the half-filling, as is well known.

By using equations (1.8)–(1.10), we rewrite E_L^{open} to obtain

$$E_L^{\text{open}} - E_L^{\text{periodic}} = f + \mathrm{O}\left(\frac{1}{L}\right) \qquad f \equiv e + 1 - \frac{\mu}{2} + \frac{h}{4} - \frac{1}{2}\varepsilon_{\mathrm{s}}(0) \tag{1.12}$$

where e denotes the ground-state energy per site for $L \to \infty$ [15], namely

$$e \equiv \frac{1}{2\pi}\int_{-k_0}^{+k_0} \mathrm{d}k\, \varepsilon_{\mathrm{c}}(k). \tag{1.13}$$

Then we find

$$m^{\mathrm{b}} = -\frac{\partial f}{\partial h} \qquad \text{and} \qquad n^{\mathrm{b}} = \frac{\partial f}{\partial \mu}. \tag{1.14}$$

Therefore, we only have to concentrate our attention on the dressed energies in order to evaluate f, and thereby m^{b} and n^{b}.

In the present paper, we discuss the following special cases,

Case 1. Half-filling case with a weak magnetic field.

Case 2. Nearly-half-filling case without magnetic field.

In section 2, we derive the boundary magnetization and the spin susceptibility for case 1. In section 3, we calculate the boundary density and the charge susceptibility for case 2. In our calculations, we adopt some techniques used by Essler [10] and by Frahm and Korepin [15, 16]. In section 4, we phenomenologically rederive the results obtained in section 2. Finally, we discuss the results thus obtained in section 5.

2. Boundary magnetization and boundary spin susceptibility

In the present section, we evaluate boundary contributions of the magnetization and the spin susceptibility at the half-filling. The half-filling case corresponds to $k_0 = \pi$. We can put μ to zero, since the number of electron is fixed.

In the present case, the integral equations (1.8) and (1.9) can be reduced to the following forms,

$$\varepsilon_{\mathrm{c}}(k) = -\frac{h}{2} - 2\cos k + \int_{-\lambda_0}^{+\lambda_0} \mathrm{d}\lambda \, a_1(\sin k - \lambda)\varepsilon_{\mathrm{s}}(\lambda) \tag{2.1}$$

and

$$\varepsilon_{\mathrm{s}}(\lambda) = h - \int_{-\pi}^{+\pi} \mathrm{d}k \, 2\cos^2 k a_1(\sin k - \lambda) - \int_{-\lambda_0}^{+\lambda_0} \mathrm{d}\lambda' \, a_2(\lambda - \lambda')\varepsilon_{\mathrm{s}}(\lambda') \tag{2.2}$$

where equation (2.2) can be obtained by substituting (1.8) into (1.9) with $k_0 = \pi$ and $\mu = 0$. By the Wiener–Hopf method, the following result can be obtained [15],

$$\tilde{y}^{+}(\omega) = G^{+}(\omega)\frac{\mathrm{i}}{\sqrt{2}}\left(\frac{h}{\omega + \mathrm{i}0} - \frac{h_0 \mathrm{e}^{-\frac{\pi}{2u}\lambda_0}}{\omega + \frac{\pi}{2u}\mathrm{i}}\right) + \begin{pmatrix}\text{less dominant terms} \\ \text{for large } \lambda_0\end{pmatrix} \tag{2.3}$$

with

$$G^{+}(\omega) = \sqrt{2\pi}\,\frac{\left(-\mathrm{i}\frac{u\omega}{e\pi}\right)^{-\mathrm{i}\frac{u\omega}{\pi}}}{\Gamma\left(\frac{1}{2} - \mathrm{i}\frac{u\omega}{\pi}\right)} \qquad h_0 = 4\sqrt{\frac{2\pi}{e}}\, I_1\left(\frac{\pi}{2u}\right) \tag{2.4}$$

where

$$\tilde{y}^{+}(\omega) = \int_0^{\infty} \mathrm{d}x \, \mathrm{e}^{\mathrm{i}x\omega} y(x) \qquad y(x) \equiv \varepsilon_{\mathrm{s}}(\lambda_0 + x). \tag{2.5}$$

Here, $I_\nu(x)$ denotes the modified Bessel function of the first kind, i.e.

$$I_\nu(x) \equiv \frac{(x/2)^\nu}{\sqrt{\pi}\,\Gamma(\nu + \frac{1}{2})} \int_0^{\pi} \mathrm{d}k \, \mathrm{e}^{x\cos k} \sin^{2\nu} k.$$

Frahm and Korepin have already obtained (2.3) in [15], although they have not shown the explicit form of $\tilde{y}^+(\omega)$. In appendix A, we briefly review this derivation. Using this expression, $\varepsilon_s(\lambda_0) = y^+(0)$ can be calculated as follows,

$$y^+(0) = -\mathrm{i}\lim_{\omega\to\infty}\omega\tilde{y}^+(\omega) = \frac{1}{\sqrt{2}}(h - h_0\mathrm{e}^{-\frac{\pi}{2u}\lambda_0}) + \begin{pmatrix}\text{less dominant terms}\\ \text{for large }\lambda_0\end{pmatrix}. \tag{2.6}$$

By solving the equation $\varepsilon_s(\lambda_0) = 0$, we can obtain the following relationship between λ_0 and h [15], apart from higher-order corrections,

$$\lambda_0 \simeq \frac{2u}{\pi}\ln\frac{h_0}{h}. \tag{2.7}$$

In order to evaluate $\varepsilon_c(k)$, we have to calculate the integral in (2.1). Now, we remark that the Fourier transformation of $\varepsilon_s(\lambda)$ takes the following form, (see equation (2.2))

$$\tilde{\varepsilon}_s(\omega) = \pi h\delta(\omega) - 2\int_{-\pi}^{+\pi}\mathrm{d}k\,\cos^2 k\frac{\mathrm{e}^{\mathrm{i}\omega\sin k}}{\mathrm{e}^{u|\omega|}+\mathrm{e}^{-u|\omega|}} + \frac{\mathrm{e}^{-u|\omega|}}{\mathrm{e}^{u|\omega|}+\mathrm{e}^{-u|\omega|}}\int_{|\lambda'|>\lambda_0}\mathrm{d}\lambda'\,\mathrm{e}^{\mathrm{i}\lambda'\omega}\varepsilon_s(\lambda'). \tag{2.8}$$

In the present paper, by the symbol $\tilde{f}(\omega)$ we describe the Fourier transformation of a function $f(\lambda)$, for example,

$$\tilde{a}_\nu(\omega) \equiv \int_{-\infty}^{+\infty}\mathrm{d}\lambda\,a_\nu(\lambda) = \mathrm{e}^{-\nu u|\omega|} \qquad (\nu > 0). \tag{2.9}$$

Taking equation (2.8) into account, we can rewrite the integral in (2.1) as follows,

$$\begin{aligned}\int_{-\lambda_0}^{+\lambda_0}\mathrm{d}\lambda\,a_1(\sin k-\lambda)\varepsilon_s(\lambda) &= \int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-\mathrm{i}\omega\sin k}\tilde{a}_1(\omega)\tilde{\varepsilon}_s(\omega) - \int_{|\lambda|>\lambda_0}\mathrm{d}\lambda\,a_1(\sin k-\lambda)\varepsilon_s(\lambda)\\ &= \frac{h}{2} - 2\int_{-\pi}^{+\pi}\mathrm{d}k'\,R(\sin k-\sin k')\cos^2 k'\\ &\quad + \int_{|\lambda'|>\lambda_0}\mathrm{d}\lambda'\,(A_2(\sin k-\lambda') - a_1(\sin k-\lambda'))\varepsilon_s(\lambda')\end{aligned} \tag{2.10}$$

where

$$A_\nu(x) \equiv \int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{e}^{-\nu u|\omega|}}{\mathrm{e}^{u|\omega|}+\mathrm{e}^{-u|\omega|}}\mathrm{e}^{-\mathrm{i}x\omega} \tag{2.11}$$

and

$$R(x) \equiv \int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{e}^{-\mathrm{i}x\omega}}{\mathrm{e}^{2u|\omega|}+1}(= A_1(x)). \tag{2.12}$$

We remark that the relationship

$$A_{n+1}(x) + A_{n-1}(x) = a_n(x) \tag{2.13}$$

holds. Especially, we find that

$$A_2(x) - a_1(x) = -A_0(x) = -\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{e}^{\mathrm{i}x\omega}}{2\cosh(u\omega)} = \frac{-1}{4u}\frac{1}{\cosh(\frac{\pi}{2u}x)}. \tag{2.14}$$

We substitute (2.10) into (2.1) to obtain

$$\varepsilon_c(k) = -2\cos k - 2\int_{-\pi}^{+\pi}\mathrm{d}k'\,R(\sin k-\sin k')\cos^2 k' + \mathcal{I}(k) \tag{2.15}$$

using the relation (2.14), where

$$\mathcal{I}(k) \equiv -\frac{1}{4u}\int_{|\lambda|>\lambda_0} \mathrm{d}\lambda \, \frac{\varepsilon_{\mathrm{s}}(\lambda)}{\cosh\frac{\pi}{2u}(\sin k - \lambda)}. \tag{2.16}$$

We evaluate the leading term with respect to h (~ 0). According the the relationship (2.7), λ_0 is extremely large for small h. Taking this fact into account, we can evaluate $\mathcal{I}(k)$ as follows,

$$\begin{aligned}\mathcal{I}(k) &= \frac{-1}{4u}\int_0^\infty \mathrm{d}\nu \left(\frac{1}{\cosh\frac{\pi}{2u}(\lambda_0+\nu-\sin k)} + \frac{1}{\cosh\frac{\pi}{2u}(\lambda_0+\nu+\sin k)}\right)\varepsilon_{\mathrm{s}}(\lambda_0+\nu)\\ &\simeq \frac{-1}{2u}\int_0^\infty \mathrm{d}\nu \left(\exp\left(\frac{-\pi}{2u}(\lambda_0+\nu-\sin k)\right)\right.\\ &\quad \left.+\exp\left(\frac{-\pi}{2u}(\lambda_0+\nu+\sin k)\right)\right) y(\nu)\\ &= -\frac{1}{u}\cosh\left(\frac{\pi \sin k}{2u}\right)\mathrm{e}^{-\frac{\pi}{2u}\lambda_0}\,\tilde{y}^{+}\left(\frac{\mathrm{i}\pi}{2u}\right).\end{aligned} \tag{2.17}$$

Using equations (2.3) and (2.7), we can rewrite this formula to obtain the leading term with respect to h as follows,

$$\mathcal{I}(k) = -\frac{1}{u}\cosh\left(\frac{\pi \sin k}{2u}\right)\sqrt{\frac{\pi}{2e}}\,\frac{u}{\pi}\,\frac{h^2}{h_0} + \mathrm{o}(h^2). \tag{2.18}$$

From equations (1.13), (2.15) and (2.18), we evaluate the quantity e in the following way,

$$e = e_0 - \frac{1}{8\pi}\frac{I_0(\frac{\pi}{2u})}{I_1(\frac{\pi}{2u})}h^2 + \mathrm{o}(h^2) \tag{2.19}$$

with

$$e_0 = -2\int_{-\infty}^{+\infty} \mathrm{d}\omega \, \frac{J_0(\omega)J_1(\omega)}{\omega(\mathrm{e}^{2u|\omega|}+1)} \tag{2.20}$$

where $J_n(x)$ denotes the Bessel function of the first kind, namely

$$J_n(x) \equiv \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}k \, \cos(x\sin k - nk).$$

Here, e_0 denotes the ground-state energy at half-filling without magnetic field [14].

Before going ahead in our calculations, we give a comment. Since e denotes the ground-state energy per site in the bulk, we can derive the magnetization and the spin susceptibility in the bulk as follows,

$$m = -\frac{\partial e}{\partial h} \simeq \frac{1}{4\pi}\frac{I_0(\frac{\pi}{2u})}{I_1(\frac{\pi}{2u})}h \tag{2.21}$$

$$\chi_{\mathrm{s}} = \frac{\partial m}{\partial h} \simeq \frac{1}{4\pi}\frac{I_0(\frac{\pi}{2u})}{I_1(\frac{\pi}{2u})} \tag{2.22}$$

in the limit $h \to 0$. As is well known, this result has been obtained in another way [11, 12]. (This quantity does not depend on the boundary condition.)

Next, we evaluate $\varepsilon_{\mathrm{s}}(0)$. For this purpose, we calculate the integral in the following equation, (see equation (2.2))

$$\varepsilon_{\mathrm{s}}(0) = h - h_{\mathrm{c}} - \int_{-\lambda_0}^{+\lambda_0} \mathrm{d}\lambda \, a_2(\lambda)\varepsilon_{\mathrm{s}}(\lambda). \tag{2.23}$$

Here, h_c is defined by

$$h_c = \int_{-\pi}^{+\pi} dk\, 2\cos^2 k\ a_1(\sin k) = 4\left(\sqrt{u^2+1} - u\right) \tag{2.24}$$

and denotes the critical field, at which the magnetization is saturated. These kinds of critical fields in various solvable models have been discussed in detail by one of the present authors (MS) [17]. We evaluate $\varepsilon_s(0)$ as follows,

$$\begin{aligned}\varepsilon_s(0) &= h - h_c - \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \tilde{a}_2(\omega)\tilde{\varepsilon}_s(\omega) + \int_{|\lambda|>\lambda_0} d\lambda\, a_2(\lambda)\varepsilon_s(\lambda) \\ &= \frac{h}{2} - 2e_1 - 2\int_{\lambda_0}^{\infty} d\lambda\, (A_3(\lambda) - a_2(\lambda))\varepsilon_s(\lambda)\end{aligned} \tag{2.25}$$

with

$$e_1 \equiv \int_{-\pi}^{+\pi} dk \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\cos^2 k e^{i\omega \sin k}}{e^{u|\omega|} + e^{-u|\omega|}}. \tag{2.26}$$

In this calculation, we have used equation (2.8). As preliminaries in the following calculations, we asymptotically expand $A_n(\lambda)$ for $\lambda \gg 1$,

$$A_x(\lambda) = \frac{1}{2u} G_x\left(\frac{\lambda}{2u}\right) = \frac{u}{2\pi}\frac{x}{\lambda^2} + O\left(\frac{1}{\lambda^4}\right) \tag{2.27}$$

where

$$\begin{aligned} G_x(\lambda) &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega\lambda} \frac{e^{-x\frac{|\omega|}{2}}}{2\cosh\frac{\omega}{2}} = \frac{1}{\pi}\,\mathrm{Re}\left(\beta\left(\frac{1+x}{2} + i\lambda\right)\right) \\ \beta(z) &\equiv \frac{1}{2}\left(\psi\left(\frac{1+z}{2}\right) - \psi\left(\frac{z}{2}\right)\right) \qquad \psi(z) = \frac{d}{dz}\ln\Gamma(z). \end{aligned} \tag{2.28}$$

Taking equations (2.13), (2.5) and (2.27) into account, we evaluate (2.25) as follows

$$\begin{aligned}\varepsilon_s(0) &= \frac{h}{2} - 2e_1 + 2\int_0^{\infty} d\nu\, A_1(\nu+\lambda_0)y(\nu) \\ &= \frac{h}{2} - 2e_1 + \frac{u}{\pi}\int_0^{\infty} d\nu \left(\frac{1}{(\nu+\lambda_0)^2} + O\left(\frac{1}{(\nu+\lambda_0)^4}\right)\right).\end{aligned} \tag{2.29}$$

Moreover, by the formula (the Laplace transformation),

$$\frac{\Gamma(\alpha+1)}{(\nu+\lambda_0)^{\alpha+1}} = \int_0^{\infty} dt e^{-\nu t} e^{-\lambda_0 t} t^{\alpha} \qquad \text{for } \mathrm{Re}(\alpha) > -1 \tag{2.30}$$

we find that

$$\int_0^{\infty} d\nu \frac{1}{(\nu+\lambda_0)^2} y(\nu) = \int_0^{\infty} dt\, e^{-\lambda_0 t} t \tilde{y}^+(it) = \frac{h}{\lambda_0} + \left(\begin{matrix}\text{higher order terms}\\ \text{with respect to } h\end{matrix}\right). \tag{2.31}$$

In evaluating the integral, we have expanded $\tilde{y}^+(\omega)$ around $\omega = 0$, namely

$$\tilde{y}^+(\omega) = \frac{ih}{\omega} + (\text{less dominant terms}) \qquad \text{for } \omega \sim 0 \tag{2.32}$$

since the leading contribution to the integral comes from the region around $t = 0$ due to the strongly dumping factor $e^{-\lambda_0 t}$. This technique has also been used in [10]. Then we have

$$\varepsilon_s(0) = \frac{h}{2} - 2e_1 - \frac{h}{2}\frac{1}{\ln(h/h_0)} + o\left(\frac{h}{\ln h}\right). \tag{2.33}$$

Substituting the terms thus evaluated into f (1.12), we obtain

$$f = e_0 + \left(-\frac{1}{8\pi} \frac{I_0(\frac{\pi}{2u})}{I_1(\frac{\pi}{2u})} h^2 + \mathrm{o}(h^2) \right) + 1 + e_1 + \left(\frac{h}{4} \frac{1}{\ln(h/h_0)} + \mathrm{o}\left(\frac{h}{\ln h} \right) \right). \tag{2.34}$$

Deriving f, we can obtain the boundary magnetization and the boundary susceptibility as follows,

$$m^{\mathrm{b}} = -\frac{\partial f}{\partial h} \simeq -\frac{1}{4} \frac{1}{\ln(h/h_0)} \tag{2.35}$$

and

$$\chi_{\mathrm{s}}^{\mathrm{b}} = \frac{\partial m^{\mathrm{b}}}{\partial h} \simeq \frac{1}{4h(\ln(h/h_0))^2} \tag{2.36}$$

for small h.

By the same way, we can evaluate the boundary magnetization and the boundary susceptibility for the arbitrary-filling case with $u \gg 1$, to obtain the same results as (2.35) and (2.36), apart from the definition of h_0.

3. Boundary density and boundary charge susceptibility

In the present section, we discuss the boundary contributions of the density and the charge susceptibility (compressibility) for $h = 0$, namely $\lambda_0 = \infty$.

In the present case, the integral equations (1.8) and (1.9) can be reduced to the following form,

$$\varepsilon_{\mathrm{c}}(k) = \mu - 2\cos k + \int_{-\infty}^{+\infty} \mathrm{d}\lambda\, a_1(\sin k - \lambda)\varepsilon_{\mathrm{s}}(\lambda) \tag{3.1}$$

$$\varepsilon_{\mathrm{s}}(\lambda) = \int_{-k_0}^{+k_0} \mathrm{d}k\, \cos k a_1(\lambda - \sin k)\varepsilon_{\mathrm{c}}(k) - \int_{-\infty}^{+\infty} \mathrm{d}\lambda'\, a_2(\lambda - \lambda')\varepsilon_{\mathrm{s}}(\lambda'). \tag{3.2}$$

By the Fourier transformation of equation (3.2), we can obtain the following equation,

$$\tilde{\varepsilon}_{\mathrm{s}}(\omega) = \frac{\mathrm{e}^{-u|\omega|}}{1 + \mathrm{e}^{-2u|\omega|}} \int_{-k_0}^{+k_0} \mathrm{d}k\, \cos k \mathrm{e}^{\mathrm{i}\omega \sin k} \varepsilon_{\mathrm{c}}(k). \tag{3.3}$$

Using equations (3.1) and (3.3), we have

$$\varepsilon_{\mathrm{c}}(k) = \mu - 2\cos k + \int_{-k_0}^{+k_0} \mathrm{d}k'\, R(\sin k - \sin k') \cos k' \varepsilon_{\mathrm{c}}(k'). \tag{3.4}$$

Moreover, we can rewrite this equation into the following form,

$$\varepsilon_{\mathrm{c}}(k) = \mu - 2\cos k - 2\int_{-\pi}^{+\pi} \mathrm{d}k'\, R(\sin k - \sin k') \cos^2 k' + \mathcal{J}(k) \tag{3.5}$$

with

$$\mathcal{J}(k) \equiv -\int_{k_0<|k'|<\pi} \mathrm{d}k'\, R(\sin k - \sin k') \cos k' \varepsilon_{\mathrm{c}}(k'). \tag{3.6}$$

We discuss the nearly half-filling case, namely $0 < \pi - k_0 \ll 1$. We find that $\mathcal{J}(k)$ is of the order $(\pi - k_0)^2$ at most, because of the condition $\varepsilon_{\mathrm{c}}(k_0) = 0$. Taking this fact into account, we can derive the following,

$$\varepsilon'(k_0) = 2(1 + C_1)(\pi - k_0) + \mathrm{O}((\pi - k_0)^2) \tag{3.7}$$

and

$$\varepsilon''(k_0) = -2(1 + C_1) + \mathrm{O}((\pi - k_0)^1) \tag{3.8}$$

with

$$C_1 \equiv \int_{-\pi}^{+\pi} \mathrm{d}k\ \sin k R'(\sin k). \tag{3.9}$$

Using equations (3.7) and (3.8), we can expand $\mathcal{J}(k)$ with respect to the small quantity $(\pi - k_0)$ to have

$$\mathcal{J}(k) = \tfrac{4}{3}(\pi - k_0)^3 R(\sin k)(1 + C_1) + \mathrm{O}((\pi - k_0)^4). \tag{3.10}$$

Next, we discuss the relationship between $\mu - \mu_0$ and $\pi - k_0$, where the symbol μ_0 denotes the chemical potential at the half-filling. The condition $\varepsilon_{\mathrm{c}}(k_0) = 0$ yields the relationship

$$0 = \mu - 2\cos k_0 - 2\int_{-\pi}^{+\pi} \mathrm{d}k'\ R(\sin k_0 - \sin k')\cos^2 k' + \mathcal{J}(k_0). \tag{3.11}$$

We remark that the following equation also holds,

$$0 = \mu_0 + 2 - 2\int_{-\pi}^{+\pi} \mathrm{d}k'\ R(-\sin k')\cos^2 k'. \tag{3.12}$$

Subtracting equation (3.12) from equation (3.11), we obtain

$$\begin{aligned} 0 &= \mu - \mu_0 - 2(\cos k_0 + 2) - 2\int_{-\pi}^{+\pi} \mathrm{d}k'\ (R(\sin k_0 - \sin k') - R(-\sin k')) + \mathcal{J}(k_0) \\ &= \mu - \mu_0 - \{(\pi - k_0)^2(1 + C_1) + \mathrm{O}((\pi - k_0)^3)\} \end{aligned} \tag{3.13}$$

namely, apart from higher order terms,

$$\pi - k_0 \simeq \sqrt{\frac{\mu - \mu_0}{1 + C_1}}. \tag{3.14}$$

For the later calculations, we need to evaluate the quantities $\varepsilon_{\mathrm{c}}(\pi)$, $\varepsilon'_{\mathrm{c}}(\pi)$ and $\varepsilon''_{\mathrm{c}}(\pi)$, as follows,

$$\begin{aligned} &\varepsilon_{\mathrm{c}}(\pi) = \mu - \mu_0 + \mathrm{O}((\pi - k_0)^3) = (1 + C_1)(\pi - k_0)^2 + \mathrm{O}((\pi - k_0)^3) \\ &\varepsilon'_{\mathrm{c}}(\pi) = 0 + \mathrm{O}((\pi - k_0)^3) \qquad \text{and} \qquad \varepsilon''_{\mathrm{c}}(\pi) = -2(1 + C_1) + \mathrm{O}((\pi - k_0)^3). \end{aligned} \tag{3.15}$$

Using the above results, we can evaluate e defined in equation (1.13). Expanding the upper and the lower edges in the integral region around π and $-\pi$, respectively, we have

$$e = e_0 + \mu - \frac{2}{3\pi}(1 + C_1)(1 - C_0)(\pi - k_0)^3 + \mathrm{O}((\pi - k_0)^4) \tag{3.16}$$

$$= e_0 + \mu - \frac{2}{3\pi}\frac{1 - C_0}{\sqrt{1 + C_1}}(\mu - \mu_0)^{\frac{3}{2}} + \mathrm{o}((\mu - \mu_0)^{\frac{3}{2}}) \tag{3.17}$$

where

$$C_0 \equiv \int_{-\pi}^{+\pi} \mathrm{d}k\ R(\sin k). \tag{3.18}$$

In this calculation, we have used relations in equation (3.15).

Before going further, we give a short remark. We derive the electron density and the charge susceptibility in the bulk as follows,

$$n = \frac{\partial e}{\partial \mu} \simeq 1 - \frac{1}{\pi}\frac{1 - C_0}{\sqrt{1 + C_1}}\sqrt{\mu - \mu_0} \tag{3.19}$$

$$\chi_{\mathrm{c}} = -\frac{\partial n}{\partial \mu} \simeq \frac{1}{2\pi}\frac{1 - C_0}{\sqrt{1 + C_1}}\frac{1}{\sqrt{\mu - \mu_0}} = \frac{\alpha}{1 - n} \tag{3.20}$$

where

$$\alpha \equiv \frac{1}{2\pi^2}\frac{(1-C_0)^2}{1+C_1}. \tag{3.21}$$

This form of χ_c has been obtained by another scheme in [13].

Next, we evaluate $\varepsilon_c(0)$. This quantity can be expressed in the following integral form

$$\varepsilon_c(0) = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\tilde{\varepsilon}_c(\omega) = \int_{-k_0}^{+k_0} dk\, \varepsilon_c(k)\frac{1}{4u}\frac{\cos k}{\cosh\left(\frac{\pi}{2u}\sin k\right)}. \tag{3.22}$$

Here, we have used equation (3.3) and performed the integration with respect to ω. By expanding the edges of the integral region in equation (3.22) around $k_0 = \pi$, we obtain

$$\varepsilon_s(0) = -2e_1 + \frac{1}{3u}(1+C_1)(\pi-k_0)^3 + O((\pi-k_0)^4) \tag{3.23}$$

$$= -2e_1 + \frac{1}{3u}\frac{1}{\sqrt{1+C_1}}(\mu-\mu_0)^{\frac{3}{2}} + o((\mu-\mu_0)^{\frac{3}{2}}) \tag{3.24}$$

where e_1 has been defined in equation (2.26).

Substituting the results thus obtained in f (1.12), we have

$$f = e_0 + e_1 + 1 + \frac{\mu}{2} - \frac{2}{3\pi}\frac{1-C_0}{\sqrt{1+C_1}}(1+\gamma)(\mu-\mu_0)^{\frac{3}{2}} + o((\mu-\mu_0)^{\frac{3}{2}}) \tag{3.25}$$

where

$$\gamma \equiv \frac{\pi}{4u}\frac{1}{1-C_0}. \tag{3.26}$$

Then, we calculate the electron density and the charge susceptibility in the boundary as follows,

$$n^b = \frac{\partial f}{\partial \mu} \simeq \frac{1}{2} - \frac{1}{\pi}\frac{1-C_0}{\sqrt{1+C_1}}(1+\gamma)\sqrt{\mu-\mu_0} \tag{3.27}$$

and

$$\chi_c^b = -\frac{\partial n^b}{\partial \mu} \simeq \frac{1}{2\pi}\frac{1-C_0}{\sqrt{1+C_1}}(1+\gamma)\frac{1}{\sqrt{\mu-\mu_0}} = \frac{\alpha(1+\gamma)}{1-n}. \tag{3.28}$$

4. Phenomenological derivation of the boundary magnetization

In section 2, we have shown that the boundary magnetization is proportional to $-1/\ln h$ for a small magnetic field h. In the present section, we rederive the result phenomenologically, and discuss the meaning of the logarithmic dependence.

In the present model with open boundaries, finite-size corrections for the energy spectrum of the spin sector are given by [7]

$$E = \frac{\pi v}{L}\left(\frac{1}{2}\frac{(\Delta M)^2}{\xi^2} + N^+ - \frac{1}{24}\right) + o\left(\frac{1}{L}\right) \tag{4.1}$$

where ΔM takes integers and N^+ takes positive integers. The degeneracy with respect to N^+ is given by the partition number $P(N^+)$. We have already subtracted the contributions of orders L^1 and L^0 from the ground-state energy. The quantity ΔM corresponds to the deviation of the total magnetization (z-component) from its ground-state value. The quantity ξ is a function of the external field h, and takes $1/\sqrt{2}$ for $h = 0$. This means that the spin sector of the Hubbard model with open boundaries is described by the chiral $SU(2)$ Kac–Moody algebra (level 1). (If the Hubbard with open boundaries is defined in a chain with length L, the corresponding chiral field lives in a periodic chain with length $2L$.)

The finite-size scaling form (4.1) yields the following partition function

$$Z = \frac{1}{\eta(q)} \sum_{N\in\mathbb{Z}} q^{\frac{N^2}{2\xi^2}} \qquad q \equiv \exp\left(-\frac{\pi v}{TL}\right). \tag{4.2}$$

By the Poisson sum formula, we can rewrite the above partition function into the following form

$$Z = \frac{\xi}{\eta(p)} \sum_{n\in\mathbb{Z}} p^{\frac{\xi^2 n^2}{2}} \qquad p \equiv \exp\left(-\frac{4\pi TL}{v}\right). \tag{4.3}$$

Here, we have defined $\eta(q)$ by

$$\eta(q) \equiv q^{\frac{1}{24}} \prod_{n=1}^{\infty} (1 - q^n). \tag{4.4}$$

From equation (4.1), we can read off the susceptibility per site in the relevant system with open boundaries as $\chi = \xi^2/(\pi v)$. Therefore, using the bulk quantity χ, we can describe ξ as follows:

$$\xi(h) = \sqrt{\pi v \chi(h)}. \tag{4.5}$$

We find that this relation holds not only in the periodic boundary case but also in the open boundary case, as it should be. In quantum systems described by the $SU(2)$ Kac–Moody algebra (level 1), the susceptibility universally behaves as

$$\chi(h) = \frac{1}{2\pi v}\left(1 + \frac{1}{2}\frac{1}{\ln 1/h}\right) + \mathrm{o}\left(\frac{1}{\ln 1/h}\right) \tag{4.6}$$

for a small h [20]. (This form of χ has been derived under the periodic boundary condition [20]. However, equation (4.6) holds even in the open-boundary case since the bulk quantity χ does not depend on the boundary condition.) Then, we substitute (4.6) into (4.5) to obtain

$$\xi(h) = \frac{1}{\sqrt{2}}\left(1 + \frac{1}{4}\frac{1}{\ln 1/h}\right) + \mathrm{o}\left(\frac{1}{\ln 1/h}\right). \tag{4.7}$$

Using the partition function (4.3), we can evaluate the part of order L^0 in the free energy, as follows,

$$f(h) = -T \ln \xi(h). \tag{4.8}$$

Therefore, the singular part of the boundary free energy can be obtained as

$$f_{\mathrm{boundary}} \equiv f(h) - f(0) = -T \ln\left(\frac{\xi(h)}{\xi(0)}\right). \tag{4.9}$$

On the other hand, the finite-size-scaling argument yields

$$f_{\mathrm{boundary}} = T f_{\mathrm{s}}(T^{-1}h; g(t)) \tag{4.10}$$

where f_{s} denotes a scaling function and $g(t)$ corresponds to the renormalized coupling constant of a perturbational interaction due to the existence of boundaries. Here, we have taken e^t as T^{-1}. For the detailed derivation, see appendix B. Now, we take the scaling limit $h \to 0$ keeping $T^{-1}h$ unity. Then, the boundary free energy takes the following form,

$$f_{\mathrm{boundary}} = h f_{\mathrm{s}}(1; g(\ln 1/h)) \equiv h\Phi(g(\ln 1/h)). \tag{4.11}$$

In this scaling limit, from equation (4.9), we also have

$$f_{\text{boundary}} = -h \ln\left(\frac{\xi(h)}{\xi(0)}\right). \tag{4.12}$$

Comparing (4.11) with (4.12), we obtain the following relationship

$$\Phi(g(\ln 1/h)) = -\ln\left(\frac{\xi(h)}{\xi(0)}\right) = -\ln\left(1 + \frac{1}{4}\frac{1}{\ln 1/h}\right) + \mathrm{o}\left(\frac{1}{\ln 1/h}\right) \tag{4.13}$$

to have

$$f_{\text{boundary}} = \frac{1}{4}\frac{h}{\ln h} + \mathrm{o}\left(\frac{h}{\ln h}\right). \tag{4.14}$$

Then, we can calculate the boundary magnetization for a small h as follows,

$$m^{\mathrm{b}} = -\frac{\partial f_{\text{boundary}}}{\partial h} \simeq \frac{1}{4}\frac{1}{\ln 1/h}. \tag{4.15}$$

This takes the same form as what we have derived in section 2, including the prefactor.

This logarithmic dependence suggests that there exists a (spatially) localized perturbational interaction described by

$$\delta\mathcal{H} = -g\hat{\phi} \tag{4.16}$$

where $\hat{\phi}$ denotes the so-called boundary operator [21] and has the dimensionality 1. When such an operator exists, we can formally derive the form of the renormalized coupling $g(\ln 1/h)$ to obtain

$$g(\ln 1/h) = \frac{g}{1 - (C/2)g\ln 1/h} = \frac{2/C}{\ln h} + \mathrm{o}\left(\frac{1}{\ln h}\right) \qquad g(0) \equiv g \tag{4.17}$$

with a constant C. For the detailed derivation, see appendix B. If $\Phi(x) \propto x$ for $x \sim 0$, we can obtain

$$f_{\text{boundary}}(h) \propto \frac{h}{\ln h}. \tag{4.18}$$

In fact, comparing (4.17) with (4.12), we find $\Phi(x) \propto \ln(1+x) \propto x$ for $x \sim 0$.

In the (chiral) $SU(2)$ Kac–Moody algebra (level 1), we have such boundary operators with the dimensionality 1, for example, the $SU(2)$-current operators [21].

5. Summary

In section 2, we have derived the boundary magnetization and the boundary spin susceptibility for the half-filling case with a weak magnetic field h. As is well known, as long as h is small, the bulk magnetization is proportional to h [11, 12]. On the other hand, the boundary magnetization is proportional to $-1/\ln h$ for small h. Similar behaviours are realized in the boundary magnetizations of the Heisenberg model and of the supersymmetric t–J model [10].

In section 3, we have derived the boundary density and the boundary charge susceptibility for the nearly-half-filling case without magnetic field. It is known that as the (bulk) filling approaches unity ($n \to 1$), the bulk charge susceptibility diverges proportional to $(1-n)^{-1}$ [13]. The boundary charge susceptibility shows the same singularity apart from the prefactor. This is the same property as that of the supersymmetric t–J model.

We expect that we can treat other cases in the one-dimensional Hubbard model with boundaries, for example, the nearly half-filling case with a weak magnetic field, the negative-u case (e.g. [19]) etc using our scheme based on the dressed energies.

Appendix A.

In the present section, we briefly explain how to derive $\tilde{y}^+(\omega)$ (2.3).

Using equation (2.8), we can write the integral equation for $\varepsilon_s(\lambda)$ in section 2, as follows,

$$\varepsilon_s(\lambda) = \varepsilon_s^{(0)}(\lambda) + \int_{|\mu|>\lambda_0} \mathrm{d}\mu\, R(\lambda-\mu)\varepsilon_s(\mu) \tag{A.1}$$

where the Fourier transformation of $\varepsilon_s^{(0)}(\lambda)$ takes the following form

$$\tilde{\varepsilon}_s^{(0)}(\omega) = \pi h \delta(\omega) - \int_{-\pi}^{+\pi} \mathrm{d}k\, \cos^2 k \frac{\mathrm{e}^{\mathrm{i}\omega \sin k}}{\cosh(u\omega)}. \tag{A.2}$$

When we define $y(x)$ and $y^{(0)}(x)$ by

$$y(x) \equiv \varepsilon_s(\lambda_0 + x) \qquad \text{and} \qquad y^{(0)}(x) \equiv \varepsilon_s^{(0)}(\lambda_0 + x) \tag{A.3}$$

we can rewrite equation (A.1) as follows,

$$y(x) = y^{(0)}(x) + \int_0^\infty \mathrm{d}\nu\, (R(x-\nu) + R(x+2\lambda_0+\nu))y(\nu). \tag{A.4}$$

Since $R(2\lambda_0 + \xi)$ is of order $\mathrm{O}(\lambda_0^{-2})$ for $\lambda_0 \gg 1$ and $\xi \geqslant 0$ (see equations (2.12) and (2.27)), we can solve perturbationally this integral equation by iteration, as follows,

$$y(x) = y_1(x) + y_2(x) + \cdots \tag{A.5}$$

$$y_1(x) = y^{(0)}(x) + \int_0^\infty \mathrm{d}\nu\, R(x-\nu)y_1(\nu)$$

$$y_2(x) = \int_0^\infty \mathrm{d}\nu\, R(x+2\lambda_0+\nu)y_1(\nu) + \int_0^\infty \mathrm{d}\nu\, R(x-\nu)y_2(\nu)\cdots. \tag{A.6}$$

When we evaluate the leading term of $y(x)$ with respect to large λ_0, we only have to approximate $y(x)$ by $y_1(x)$ and solve the following equation,

$$y(x) - \int_0^\infty \mathrm{d}\nu\, R(x-\nu)y(\nu) = y^{(0)}(x). \tag{A.7}$$

By the Fourier transformation, we rewrite this equation into

$$(1-\tilde{R}(\omega))\tilde{y}^+(\omega) + \tilde{y}^-(\omega) = \tilde{y}^{(0)}(\omega) \tag{A.8}$$

where

$$y^+(\omega) \equiv \int_0^{+\infty} \mathrm{d}x\, y(x)\mathrm{e}^{\mathrm{i}\omega x} \qquad \text{and} \qquad y^-(\omega) \equiv \int_{-\infty}^0 \mathrm{d}x\, y(x)\mathrm{e}^{\mathrm{i}\omega x} \tag{A.9}$$

which are analytic for $\mathrm{Im}(\omega) > 0$ and $\mathrm{Im}(\omega) < 0$, respectively.

It is known [18] that the following factorization holds,

$$1 + \mathrm{e}^{-c|\omega|} = \mathcal{G}^+\left(\frac{c\omega}{2\pi}\right)\mathcal{G}^-\left(\frac{c\omega}{2\pi}\right). \tag{A.10}$$

Here, the functions $\mathcal{G}^+(z)$ and $\mathcal{G}^-(z)$ defined by

$$\mathcal{G}^+(z) \equiv \frac{\sqrt{2\pi}\left(-\frac{iz}{e}\right)^{-iz}}{\Gamma(\frac{1}{2} - iz)} \qquad \text{and} \qquad \mathcal{G}^-(z) \equiv \mathcal{G}^+(-z) \tag{A.11}$$

which are analytic and also do not take zero, in the upper and lower complex z plain, respectively.

In the present case, since we have

$$1 - \tilde{R}(\omega) = \frac{1}{1 + \mathrm{e}^{-2u|\omega|}} \tag{A.12}$$

we can rewrite equation (A.8) into the following form,

$$(G^+(\omega))^{-1}\tilde{y}^+(\omega) + G^-(\omega)\tilde{y}^-(\omega) = Q^+(\omega) + Q^-(\omega) \tag{A.13}$$

with

$$G^\pm(\omega) \equiv \mathcal{G}^\pm\left(\frac{u\omega}{\pi}\right) \tag{A.14}$$

and

$$Q^+(\omega) + Q^-(\omega) \equiv G^-(\omega)\tilde{y}^{(0)}(\omega) = G^-(\omega)\mathrm{e}^{-\mathrm{i}\lambda_0\omega}\tilde{\varepsilon}_{\mathrm{s}}^{(0)}(\omega). \tag{A.15}$$

Here, $Q^\pm(\omega)$ are analytic for $\pm\mathrm{Im}(\omega) > 0$. Comparing the both sides in equation (A.13), we can obtain

$$\tilde{y}^+(\omega) = G^+(\omega)Q^+(\omega). \tag{A.16}$$

In the present case, we have

$$Q^+(\omega) = \frac{G^-(0)}{\omega + \mathrm{i}0}\frac{\mathrm{i}h}{2} - \mathrm{e}^{-\frac{\pi\mathrm{i}}{2u}\lambda_0}\frac{G^-\left(-\frac{\pi\mathrm{i}}{2u}\right)}{\omega + \frac{\pi\mathrm{i}}{2u}}\frac{\mathrm{i}}{u}\int_{-\pi}^{+\pi}\mathrm{d}k\,\cos^2 k\,\mathrm{e}^{\frac{\pi\mathrm{i}}{2u}\sin k} + \mathrm{O}(\mathrm{e}^{-3\frac{\pi\mathrm{i}}{2u}\lambda_0}). \tag{A.17}$$

Then, if we neglect less dominant terms for large λ_0, we obtain

$$\tilde{y}^+(\omega) \simeq G^+(\omega)\frac{\mathrm{i}}{\sqrt{2}}\left(\frac{h}{\omega + \mathrm{i}0} - \mathrm{e}^{-\frac{\pi\mathrm{i}}{2u}\lambda_0}\frac{h_0}{\omega + \frac{\pi\mathrm{i}}{2u}}\right) \qquad h_0 = 4\sqrt{\frac{2\pi}{e}}I_1\left(\frac{\pi}{2u}\right). \tag{A.18}$$

Appendix B.

In the present section, we derive equations (4.10) and (4.17), using the finite-size scaling technique and the renormalization group method.

According to the finite-size scaling hypothesis, near the critical point, the singular part of the free energy density is transformed as

$$f_{\mathrm{sing}}\left(\frac{1}{L_1}, \frac{1}{L_2}, \ldots, \frac{1}{L_d}, h, t_{\mathrm{r}}\right) = b^{-d} f_{\mathrm{sing}}\left(\frac{b}{L_1}, \frac{b}{L_2}, \ldots, \frac{b}{L_d}, b^{d-x}h, b^{\frac{1}{\nu}}t_{\mathrm{r}}\right) \tag{B.1}$$

where d denotes the dimension of the relevant system. We describe an external field and the reduced temperature by h and t_{r}, respectively. Therefore, f_{sing} can take the following form,

$$f_{\mathrm{sing}} = L_1^{-d}\tilde{f}\left(\frac{L_1}{L_2}, \ldots, \frac{L_1}{L_d}, L_1^{d-x}h, L_1^{\frac{1}{\nu}}t_{\mathrm{r}}\right) \tag{B.2}$$

with some scaling function $\tilde{f}$. Especially, for $d = 2$, we have

$$f_{\mathrm{sing}} = M^{-2}\tilde{f}\left(\frac{M}{L}, M^{2-x}h, M^{\frac{1}{\nu}}t_{\mathrm{r}}\right). \tag{B.3}$$

In terms of a quantum system on a chain, L and M are proportional to the length of the chain and to the inverse temperature(T^{-1}), respectively. We expand equation (B.3) with respect to $M/L \ll 1$ as follows,

$$f_{\mathrm{sing}} = M^{-2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{M}{L}\right)^n\tilde{f}_n(M^{2-x}h, M^{\frac{1}{\nu}}t_{\mathrm{r}}) \qquad \tilde{f}_n(y, z) \equiv \frac{\partial^n}{\partial x^n}\tilde{f}(x, y, z)\bigg|_{x=0}. \tag{B.4}$$

Then, the following scaling forms of the bulk contribution (f_{bulk}) and the boundary contribution (f_{boundary}) to the free energy density can be obtained

$$f_{\mathrm{sing}} \simeq f_{\mathrm{bulk}} + \frac{1}{L} f_{\mathrm{boundary}} \qquad L \to \infty \tag{B.5}$$

$$f_{\mathrm{bulk}} = M^{-2} \tilde{f}_0(M^{2-x}h, M^{\frac{1}{\nu}} t_{\mathrm{r}}) \qquad f_{\mathrm{boundary}} = M^{-1} \tilde{f}_1(M^{2-x}h, M^{\frac{1}{\nu}} t_{\mathrm{r}}). \tag{B.6}$$

In one-dimensional quantum systems described by the $SU(2)$ Kac–Moody algebra (discussed in section 4), $x = 1$ holds. (In fact, we can find $f_{\mathrm{bulk}} \propto h^{2/(2-x)}$ from equation (B.6) with $t_{\mathrm{r}} = 0$ and $M^{2-x}h = 1$. On the other hand, it is known [20] that f_{bulk} is proportional to h^2 in such systems.) Then, for the present critical system ($t_{\mathrm{r}} = 0$), we obtain

$$f_{\mathrm{boundary}} = T \tilde{f}_1(T^{-1}h, 0) \tag{B.7}$$

where we have replaced M^{-1} with T. Now, we introduce a parameter t by $e^t = T^{-1}$. This means that the 'lattice spacing' a (in the imaginary-time direction) is changed by $\mathrm{d}a = a\,\mathrm{d}t$ (namely $a \propto \mathrm{e}^t$). We also take a perturbational interaction into account, whose coupling constant g are renormalized to $g(t)$, by this scaling. Then, we can express the boundary free energy f_{boundary} by a scaling function f_{s} as follows,

$$f_{\mathrm{boundary}} = T f_{\mathrm{s}}(T^{-1}h; g(t)). \tag{B.8}$$

We take the scaling limit $h \to 0$ keeping $T^{-1}h$ unity. Then, equation (B.8) can be rewritten into the following form

$$f_{\mathrm{boundary}} = h f_{\mathrm{s}}(1; g(\ln 1/h)) \equiv h\Phi(g(\ln 1/h)). \tag{B.9}$$

Next, we derive the function $g(t)$. The action of the relevant model in the two-dimensional Euculidean spacetime is described by the following form,

$$S = S_0 - g \int \mathrm{d}\tau\, \phi(\tau) \tag{B.10}$$

where $\phi(\tau)$ denotes a field defined at $(0, \tau)$ in the spacetime, namely $\phi(\tau) \equiv \phi(0, \tau)$. The action in (B.10) corresponds to the Hamiltonian in (4.16). We introduce the bare coupling constant λ by $\lambda = a^{1-x} g$, where a denotes the lattice spacing introduced above and x corresponds to the dimensionality of the field. Then, the partition function can be formally written as

$$Z(\lambda) = \sum_{n=0}^{\infty} \int \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_n \frac{(\lambda a^{x-1})^n}{n!} \langle \phi(\tau_1) \cdots \phi(\tau_n) \rangle \prod_{i<j} \Theta(|\tau_i - \tau_j| - a) \tag{B.11}$$

where $\langle \cdots \rangle$ denotes the average with respect to S_0. Here, we have introduced the ultraviolet cut-off in the imaginary-time integral using the step function $\Theta(x)$. When the lattice spacing a varies as

$$a \to a + a\,\mathrm{d}t \tag{B.12}$$

we have to change the coupling constant λ as

$$\lambda \to \lambda + (1-x)\lambda\,\mathrm{d}t + \frac{C}{2}\lambda^2\,\mathrm{d}t + \mathrm{O}(\lambda^3\,\mathrm{d}t) \tag{B.13}$$

so that we can keep the partition function invariant. Here, we have used that the operator product expansion of the field ϕ takes the following form,

$$\phi(\boldsymbol{r}_a)\phi(\boldsymbol{r}_b) = \frac{C}{|\boldsymbol{r}_a - \boldsymbol{r}_a|^x} \phi(\boldsymbol{r}_b) + \cdots. \tag{B.14}$$

Then, we obtain the β function

$$\beta(t) \equiv \frac{\mathrm{d}\lambda}{\mathrm{d}t} = (1-x)\lambda + \frac{C}{2}\lambda^2 + \mathrm{O}(\lambda^3). \tag{B.15}$$

Especially, for $x = 1$ we find

$$\frac{\mathrm{d}g}{\mathrm{d}t} = \frac{C}{2} g^2 \tag{B.16}$$

where we have replaced λ by g and have neglected the higher-order terms. Then, the function $g(t)$ can be obtained as follows

$$g(t) = \frac{g}{1-(C/2)gt} \qquad g(0) \equiv g. \tag{B.17}$$

We substitute (B.17) into (B.9) to have

$$f_{\mathrm{boundary}} = h\Phi\left(\frac{g}{1-(C/2)g\ln 1/h}\right) \tag{B.18}$$

for $x = 1$.

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