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The local Tomonaga–Luttinger liquid in the one-dimensional Hubbard model with a boundary field

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Abstract. The properties of the one-dimensional Hubbard model with a boundary field are studied. In the strong-coupling limit, the compressibility and the susceptibility induced by the boundary field are evaluated using the Bethe *ansatz* equation. These quantities are governed by the density of states at the Fermi level. The results obtained from our calculations seem to suggest that the local state induced by the boundary field realizes the local Tomonaga–Luttinger liquid.

1. Introduction

Recently, the interest in one-dimensional impurity problems has been renewed, with the development of nanofabrication techniques for quantum wires. One-dimensional quantum systems are no longer subjects only of theoretical physics. In particular, investigations of impurity effects in strongly correlated quantum chains (wires), which realize Tomonaga–Luttinger liquids, have attracted much attention theoretically and experimentally. From an experimental viewpoint, the transport properties of such quantum wires with impurities are of particular interest. Theoretical attempts have been made to describe such systems, using bosonization methods, renormalization-group techniques, and so on (see, e.g., [22–24]). A model representing a strongly correlated quantum chain with an impurity has been introduced and solved exactly [25, 26]. Through these theoretical studies, it has been clarified that one-dimensional quantum systems with boundaries are closely related to impurity problems. Indeed, an interacting-electron-gas system with an impurity can be mapped onto the boundary sine–Gordon model, which is an exactly solvable model with boundaries [27, 28]. (See, e.g., references [11, 12], also.) (Here, we should remark that one-dimensional quantum systems with boundaries have received renewed interest from a mathematical point of view, as well as from such a physical point of view. Exactly solvable one-dimensional quantum systems with boundary fields have a connection with generalizations of quantum-group-invariant models; see, e.g., references [29, 30].)

In recent years, the one-dimensional Hubbard model with boundary fields has been studied from various viewpoints. The Bethe *ansatz* equation of the present model has been derived [1–5] and the integrability of the model has been discussed [6, 7]. The solutions of the Bethe *ansatz* equation have been investigated [8]. Various physical properties of the model have also been studied; see, e.g., [9, 10].

The main purpose of the present paper is to clarify a feature of an impurity problem in the Hubbard open chain with a boundary field. In this paper, we discuss the one-dimensional

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Hubbard model, described by the following Hamiltonian:

$$\mathcal{H} = -\sum_{j=1}^{L-1}\sum_{\sigma=\pm}(c_{j\sigma}^{\dagger}c_{j+1\sigma} + c_{j+1\sigma}^{\dagger}c_{j\sigma}) + 4u\sum_{j=1}^{L} n_{j+}n_{j-} + \mu\sum_{j=1}^{L}(n_{j+} + n_{j-}) - \frac{h}{2}\sum_{j=1}^{L}(n_{j+} - n_{j-}) - p(n_{1+} + n_{1-}) \qquad (0 \leqslant p). \tag{1.1}$$

Here, the symbol $c_{j\sigma}$ (or $c_{j\sigma}^{\dagger}$) denotes the annihilation (or creation) operator of an electron with spin σ at site j. The number operator of an electron is defined by $n_{j\sigma} \equiv c_{j\sigma}^{\dagger}c_{j\sigma}$. The symbol p stands for the magnitude of the boundary potential. We describe the length of the chain by L, which is assumed to take an even integer value.

The Bethe *ansatz* equation of the present model (1.1) has been derived in [2]. Recently, Bedürftig and Frahm [8] have discussed the ground-state solutions of the Bethe *ansatz* equation and have derived the spectrum of boundary bound states.

In this model, some electrons may tend to localize near the boundary due to an attractive potential at the site 1. That is, the boundary potential is expected to induce an impurity spin which almost localizes near the edge site. (Indeed, for a large p, the existence of bound states has been clarified in reference [8].) In this sense, our model resembles the Anderson model:

$$\mathcal{H} = \sum_{k,\sigma} kc_{k\sigma}^{\dagger}c_{k\sigma} + V\sum_{k,\sigma}(c_{k\sigma}^{\dagger}d_{\sigma} + d_{\sigma}^{\dagger}c_{k\sigma}) + \epsilon_d\sum_{\sigma} d_{\sigma}^{\dagger}d_{\sigma} + Ud_{+}^{\dagger}d_{+}d_{-}^{\dagger}d_{-} \tag{1.2}$$

where free conduction electrons ($c_{k\sigma}$) couple correlated electrons (d_{σ}) at an impurity site. However, we observe a significant difference between these models (1.1) and (1.2). Namely, the electrons in our model are strongly correlated while the conduction electrons have no interactions in the Anderson model. (The similarities of and the differences between the properties of these models will be discussed later; see section 5.)

In the present paper, we mainly investigate the model (1.1) with $u \gg 1$ and $p \sim \mathrm{O}(u^0)$ by evaluating the compressibility and the susceptibility induced by the boundary potential, in the ground state. For this purpose, first of all, we have to derive a formal expression for the ground-state energy as a function of the chemical potential (μ) and the magnetic field (h) (section 2). Next, we evaluate the ground-state energy in order to calculate the compressibility and the susceptibility induced by the boundary potential (section 3). In section 4, we derive the relationship between the physical quantities thus obtained and the density of states at the Fermi level. In section 5, we discuss the properties of the local states induced by the boundary potential, using the results obtained in sections 3 and 4. Comparing the properties of the models (1.1) and (1.2), we propose a conjecture regarding the local state of our model (section 5). We also evaluate the Wilson ratio within our assumption. In section 6, we briefly discuss the possibility of the experimental realization of the one-dimensional Hubbard model with magnetic impurities. Finally, we summarize the results obtained from our calculations, in section 7.

2. The formal expression for the ground-state energy

The purpose of the present section is to give a formal expression of the ground-state energy of the model (1.1), as a preliminary to our calculations.

Taking the boundary bound states [8] into account, we describe the ground-state energy E of the present model, as follows:

$$\frac{E}{L} = e + \frac{1}{L}(f + \delta f_p) + \mathrm{o}\left(\frac{1}{L}\right). \tag{2.1}$$

Here, we have described the bulk and the boundary contributions to the ground-state energy by the symbols e and $f + \delta f_p$, respectively. When the boundary potential vanishes, the boundary contribution to the ground-state energy is equal to f. That is, the energy δf_p takes the value zero for $p = 0$, and f does not depend on p. These quantities, e, f and δf_p, are given by

$$e = \int_{-k_0}^{k_0} \frac{\mathrm{d}k}{2\pi}\ \varepsilon_{\mathrm{c}}(k) \qquad f = e - \frac{1}{2}\left(\varepsilon_{\mathrm{s}}(0) - \frac{h}{2}\right) + 1 - \frac{\mu}{2} \qquad \delta f_p = \Phi_p + \Psi_p \tag{2.2}$$

respectively. Here, we have introduced Φ_p as Ψ_p, which are as follows:

$$\Phi_p \equiv \frac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\ \varepsilon_{\mathrm{c}}(k)\phi_p(k) \qquad \phi_p(k) \equiv \frac{1}{2\pi \mathrm{i}}\ \frac{\mathrm{d}}{\mathrm{d}k} \ln \frac{1 - p\mathrm{e}^{-\mathrm{i}k}}{1 - p\mathrm{e}^{+\mathrm{i}k}} \tag{2.3}$$

and

$$\Psi_p \equiv 0 \qquad \text{for region 0} \tag{2.4}$$

$$\Psi_p \equiv \epsilon_1 + \mu + \frac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\ \cos k\varepsilon_{\mathrm{c}}(k) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{-\mathrm{i}\omega \sin k} \frac{\mathrm{e}^{-u|\omega|}\cosh t\omega}{\cosh u\omega} - \frac{1}{2}\int_{|\lambda|>\lambda_0} \mathrm{d}\lambda\ \varepsilon_{\mathrm{s}}(\lambda) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{-\mathrm{i}\omega\lambda} \frac{\cosh t\omega}{\cosh u\omega} \qquad \text{for region I} \tag{2.5}$$

$$\Psi_p \equiv \epsilon_1 + \mu + \frac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\ \cos k\varepsilon_{\mathrm{c}}(k) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{-\mathrm{i}\omega \sin k} \frac{\mathrm{e}^{-u|\omega|}\cosh t\omega}{\cosh u\omega} + \frac{1}{2}\int_{|\lambda|>\lambda_0} \mathrm{d}\lambda\ \varepsilon_{\mathrm{s}}(\lambda) \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{-\mathrm{i}\omega\lambda} \frac{\cosh(2u - t)\omega}{\cosh u\omega} \qquad \text{for region II} \tag{2.6}$$

$$\Psi_p \equiv \epsilon_1 + \epsilon_2 + 2\mu + \frac{1}{2}\int_{-k_0}^{k_0} \mathrm{d}k\ \cos k\varepsilon_{\mathrm{c}}(k)(a_t(\sin k) - a_{t-2u}(\sin k)) \qquad \text{for region III} \tag{2.7}$$

with

$$t \equiv \frac{1}{2}(p - p^{-1}) \qquad \epsilon_1 \equiv -2t \qquad \epsilon_2 \equiv -2\sqrt{1 + (t - 2u)^2} \tag{2.8}$$

$$a_x(\lambda) \equiv \frac{1}{\pi}\frac{x}{\lambda^2 + x^2} \qquad (x > 0). \tag{2.9}$$

Here, regions 0, I, II and III correspond to $0 \leqslant p < 1$, $1 < p < p_1$ $(\equiv u + \sqrt{1 + u^2})$, $p_1 < p < p_2$ $(\equiv 2u + \sqrt{1 + (2u)^2})$ and $p_2 < p$, respectively [8]. The symbols $\varepsilon_{\mathrm{c}}(k)$ and $\varepsilon_{\mathrm{s}}(\lambda)$ denote the dressed energies of the charge and spin sectors, respectively, which are defined by the following integral equations (see, e.g., [13, 14]):

$$\varepsilon_{\mathrm{c}}(k) = \mu - \frac{h}{2} - 2\cos k + \int_{-\lambda_0}^{\lambda_0} \mathrm{d}\lambda\ a_u(\sin k - \lambda)\varepsilon_{\mathrm{s}}(\lambda) \tag{2.10}$$

$$\varepsilon_{\mathrm{s}}(\lambda) = h + \int_{-k_0}^{k_0} \mathrm{d}k\ \cos k a_u(\lambda - \sin k)\varepsilon_{\mathrm{c}}(k) + \int_{-\lambda_0}^{\lambda_0} \mathrm{d}\lambda'\ a_{2u}(\lambda - \lambda')\varepsilon_{\mathrm{s}}(\lambda'). \tag{2.11}$$

We can determine the parameters k_0 and λ_0 from

$$\varepsilon_{\rm c}(k_0) = 0 \qquad \varepsilon_{\rm s}(\lambda_0) = 0. \tag{2.12}$$

For detailed derivations of the expression for the ground-state energy, refer to, e.g., [10, 12].

In our discussions, we recognize E as a function *not* of the electron number or the magnetization *but* of the chemical potential and the magnetic field. Therefore, the number of electrons (N) and the magnetization (M) are given in the following way:

$$\frac{N}{L} = n + \frac{1}{L}(n^{\rm b} + \delta n_p) + {\rm o}\left(\frac{1}{L}\right) \tag{2.13}$$

with

$$n = \frac{\partial e}{\partial \mu} \qquad n^{\rm b} = \frac{\partial f}{\partial \mu} \qquad \delta n_p = \frac{\partial(\delta f_p)}{\partial \mu} \tag{2.14}$$

and

$$\frac{M}{L} = m + \frac{1}{L}(m^{\rm b} + \delta m_p) + {\rm o}\left(\frac{1}{L}\right) \tag{2.15}$$

with

$$m = -\frac{\partial e}{\partial h} \qquad m^{\rm b} = -\frac{\partial f}{\partial h} \qquad \delta m_p = -\frac{\partial(\delta f_p)}{\partial h}. \tag{2.16}$$

3. Physical quantities induced by the boundary potential

In the present section, we evaluate the ground-state energy of the present model to derive the physical quantities. We only discuss the case with $u \gg 1$ and $p \sim {\rm O}(u^0)$.

In the strong-coupling limit, the integral equations of the dressed energies take the following forms [14]:

$$\varepsilon_{\rm c}(k) = \mu - \frac{h}{2} - 2\cos k + \int_{-B}^{B} {\rm d}\lambda\ a_1(\lambda)\varepsilon_{\rm s}(\lambda) + {\rm O}\left(\frac{1}{u^2}\right) \tag{3.1}$$

$$\varepsilon_{\rm s}(\lambda) = h - \pi h_{\rm c} a_1(\lambda) - \int_{-B}^{B} {\rm d}\lambda'\ a_2(\lambda - \lambda')\varepsilon_{\rm s}(\lambda') + {\rm O}\left(\frac{1}{u^2}\right) \tag{3.2}$$

with

$$\varepsilon_{\rm c}(Q) = 0 \qquad \varepsilon_{\rm s}(B) = 0. \tag{3.3}$$

Here, we have defined $h_{\rm c}$ by

$$h_{\rm c} = -\frac{1}{u\pi}\int_{-Q}^{Q} {\rm d}k\ \cos k\varepsilon_{\rm c}(k). \tag{3.4}$$

For $h = h_{\rm c}$, all of the spins are pointing up (i.e. $B = 0$).

In the above expressions, the symbol $\varepsilon_{\rm s}(\lambda)$ corresponds to $\varepsilon_{\rm s}(u\lambda)$ defined in the previous section. Moreover, the (Q, B) correspond to the $(k_0, \lambda_0/u)$.

By the Wiener–Hopf method, $\varepsilon_{\rm s}(\lambda)$ can be evaluated [14] for $h \ll 1$; it takes the following form:

$$\tilde{y}^+(\omega) \simeq \frac{\rm i}{\sqrt{2}} h G^+(\omega)\left(\frac{1}{\omega + {\rm i}0} - \frac{1}{\omega + {\rm i}\pi/2}\right) \qquad {\rm e}^{-(\pi/2)B} \simeq \frac{h}{h_0} \tag{3.5}$$

with

$$y(x) \equiv \varepsilon_s(B+x) \qquad \tilde{y}^+(\omega) \equiv \int_0^\infty \mathrm{d}x\ y(x)\mathrm{e}^{\mathrm{i}\omega x} \qquad h_0 \equiv h_c\sqrt{\frac{\pi^3}{2e}}$$

and

$$G^+(\omega) = \frac{\sqrt{2\pi}(-\mathrm{i}\omega/e\pi)^{-\mathrm{i}\omega/\pi}}{\Gamma(\frac{1}{2}-\mathrm{i}\omega/\pi)} \tag{3.6}$$

where the symbol $\simeq$ means that we neglect higher-order corrections of a small h and a large u. We can also obtain the explicit form of $\varepsilon_c(k)$ as follows:

$$\varepsilon_c(k) = 2\cos Q - 2\cos k + \mathrm{O}\left(\frac{1}{u^2}\right) \tag{3.7}$$

with

$$\mu = 2\cos Q + h_c\left\{\frac{1}{2}\ln 2 + \frac{1}{\pi^2}\left(\frac{h}{h_c}\right)^2 + \mathrm{o}(h^2)\right\} + \mathrm{O}\left(\frac{1}{u^2}\right). \tag{3.8}$$

Here, we remark that h_c is of order $1/u$. Within our discussions, we recognize that h/h_c is of order u^0. Using the explicit forms of the dressed energies (3.5) and (3.7), we can evaluate the ground-state energies.

First, we evaluate e and f, obtaining

$$e = \frac{2}{\pi}(Q\cos Q - \sin Q) + \mathrm{O}\left(\frac{1}{u^2}\right) \tag{3.9}$$

$$f = e + 1 - \frac{\mu}{2} + \frac{\pi}{8}h_c + \left(\frac{h}{4}\frac{1}{\ln(h/h_0)} + \mathrm{o}\left(\frac{h}{\ln h}\right)\right) + \mathrm{O}\left(\frac{1}{u^2}\right). \tag{3.10}$$

We differentiate e with respect to μ and h (see equations (2.14) and (2.16)), and have

$$n = \frac{Q}{\pi} + \mathrm{O}\left(\frac{1}{u}\right) \qquad m = \frac{2Q}{\pi^3}\left(\frac{h}{h_c} + \mathrm{o}(h)\right) + \mathrm{O}\left(\frac{1}{u}\right). \tag{3.11}$$

In this derivation, we have to take the relationship (3.5) into account. Here, we have rederived the relation

$$m = \frac{2n}{\pi^2}\frac{h}{h_c} \tag{3.12}$$

for a small h, which was obtained in reference [15]. Similarly, we can also obtain the following results:

$$n^b = n - \frac{1}{2} + \mathrm{O}\left(\frac{1}{u}\right) \qquad m^b = \left(\frac{1}{4}\frac{1}{\ln(h_0/h)} + \mathrm{o}\left(\frac{h}{\ln h}\right)\right) + \mathrm{O}\left(\frac{1}{u}\right). \tag{3.13}$$

This boundary magnetization (m^b) takes the same form as those for other one-dimensional magnets, e.g. the antiferromagnetic Heisenberg model [16], the supersymmetric t–J model [12], and the half-filled Hubbard model [10]. For detailed discussions of the universal behaviour of the boundary magnetization, see reference [17].

Next, we discuss the contributions induced by the boundary potential. We remark that each of the parameters p_1 and p_2 is of order u for $u \gg 1$. Therefore, as long as we are studying the case with $u \gg 1$ and $p \sim \mathrm{O}(u^0)$, we only have to consider regions 0 and I.

3.1. $0 \leqslant p < 1$ *(region 0)*

In this region, we evaluate δf_p, obtaining

$$\delta f_p = \Phi_p = 2\int_0^Q \mathrm{d}k\ (\cos Q - \cos k)\phi_p(k) + \mathrm{O}\left(\frac{1}{u^2}\right). \tag{3.14}$$

By differentiating δf_p with respect to μ or h, we obtain the contributions induced by the boundary potential as follows:

$$\delta n_p = \varphi_p(n\pi) + \mathrm{O}\left(\frac{1}{u}\right) \tag{3.15}$$

$$\delta m_p = \frac{2}{\pi^2}\varphi_p(n\pi)\left(\frac{h}{h_\mathrm{c}} + \mathrm{o}(h)\right) + \mathrm{O}\left(\frac{1}{u}\right) \tag{3.16}$$

with

$$\varphi_p(Q) = \int_0^Q \mathrm{d}k\ \phi_p(k). \tag{3.17}$$

3.2. $1 < p$ *(region I)*

In this region, δf_p takes the following form:

$$\delta f_p = \Phi_p + \Psi_p \tag{3.18}$$

with

$$\Psi_p = \epsilon_1 + \mu + \frac{1}{u}\frac{\ln 2}{2\pi}(Q\cos Q - \sin Q) - h_\mathrm{c}\left(\frac{1}{\pi^2}\left(\frac{h}{h_\mathrm{c}}\right)^2 + \mathrm{o}(h^2)\right) + \mathrm{O}\left(\frac{1}{u^2}\right). \tag{3.19}$$

Here, Φ_p takes the same form as in region 0. We differentiate δf_p with respect to μ or h, obtaining the following results:

$$\delta n_p = 1 + \varphi_p(n\pi) + \mathrm{O}\left(\frac{1}{u}\right) \tag{3.20}$$

$$\delta m_p = \frac{2}{\pi^2}(1 + \varphi_p(n\pi))\left(\frac{h}{h_\mathrm{c}} + \mathrm{o}(h)\right) + \mathrm{O}\left(\frac{1}{u}\right). \tag{3.21}$$

Here, we remark that in both regions the relationship

$$\delta m_p = \frac{2\delta n_p}{\pi^2}\frac{h}{h_\mathrm{c}} \tag{3.22}$$

holds for a small h. This relation is similar to equation (3.12).

Now, we also evaluate boundary potential contributions to the compressibility $\delta\chi_p^\mathrm{c}$ and the susceptibility $\delta\chi_p^\mathrm{s}$. Ignoring higher-order corrections of $1/u$, we can derive the following results:

$$\delta\chi_p^\mathrm{c} \equiv -\frac{\partial(\delta n_p)}{\partial\mu} = \pi\phi_p(n\pi)\chi_0^\mathrm{c} \tag{3.23}$$

$$\delta\chi_p^\mathrm{s} \equiv \left.\frac{\partial(\delta m_p)}{\partial h}\right|_{h=0} = \begin{cases} \dfrac{1}{n}\phi_p(n\pi)\chi_0^\mathrm{s} & 0 \leqslant p < 1 \\ \dfrac{1}{n}(1+\phi_p(n\pi))\chi_0^\mathrm{s} & 1 < p \end{cases} \tag{3.24}$$

with

$$\chi_0^\mathrm{c} \equiv -\frac{\partial n}{\partial\mu} = \frac{1}{2\pi\sin n\pi} \qquad \chi_0^\mathrm{s} \equiv \left.\frac{\partial m}{\partial h}\right|_{h=0} = \frac{2n}{\pi^2 h_\mathrm{c}}. \tag{3.25}$$

4. Relationships between physical quantities and the density of states at the Fermi level

In the present section, we derive the relationship between the physical quantities obtained in section 3 and the density of states at the Fermi level.

At first, we concentrate on the density of states $D_{\rm F}^{\rm c\,(s)}$ at the Fermi level of the quasiparticles in the charge (spin) sector. Such a density of states is known to be described by the distribution function of the roots of the Bethe *ansatz* equation; see, e.g., reference [18]. In the present model, we have

$$D_{\rm F}^{\rm c} = \frac{1}{2\pi v_{\rm c}}\left(1+\frac{1}{L}\left(\frac{\rho_{\rm b}(k_0)}{\rho(k_0)}+\frac{\delta\rho_p(k_0)}{\rho(k_0)}\right)+{\rm o}\left(\frac{1}{L}\right)\right) \tag{4.1}$$

$$D_{\rm F}^{\rm s} = \frac{1}{2\pi v_{\rm s}}\left(1+\frac{1}{L}\left(\frac{\sigma_{\rm b}(\lambda_0)}{\sigma(\lambda_0)}+\frac{\delta\sigma_p(\lambda_0)}{\sigma(\lambda_0)}\right)+{\rm o}\left(\frac{1}{L}\right)\right). \tag{4.2}$$

Here, the symbols $\rho(k)$, $\sigma(\lambda)$, etc, are defined through the distribution functions of the roots $\rho_{\rm c}(k)$ and $\rho_{\rm s}(\lambda)$ in the charge and the spin sector, respectively, as follows:

$$\rho_{\rm c}(k) = \rho(k)+\frac{1}{L}(\rho_{\rm b}(k)+\delta\rho_p(k))+{\rm o}\left(\frac{1}{L}\right) \tag{4.3}$$

$$\rho_{\rm s}(\lambda) = \sigma(\lambda)+\frac{1}{L}(\sigma_{\rm b}(\lambda)+\delta\sigma_p(\lambda))+{\rm o}\left(\frac{1}{L}\right). \tag{4.4}$$

The symbols ρ and σ denote the distribution functions of the roots in the thermodynamic limit, and $\rho_{\rm b}+\delta\rho_p$ and $\sigma_{\rm b}+\delta\sigma_p$ correspond to the boundary contributions to the distribution functions of the roots. Each of $\delta\rho_p$ and $\delta\sigma_p$ takes the value zero for $p=0$, and $\rho_{\rm b}$ and $\sigma_{\rm b}$ do not depend on p. The integral equations for the distribution functions of the roots of the Bethe *ansatz* equation have already been derived in reference [8]. We give the integral equations in appendix A.

The relationships (4.1) and (4.2) yield

$$\frac{\delta D_p^{\rm c}}{D_0^{\rm c}} = \frac{\delta\rho_p(k_0)}{\rho(k_0)} \qquad \frac{\delta D_p^{\rm s}}{D_0^{\rm s}} = \frac{\delta\sigma_p(\lambda_0)}{\sigma(\lambda_0)}. \tag{4.5}$$

Here, the symbol $D_0^{\rm c\,(s)}$ denotes the density of states at the Fermi level in the thermodynamic limit. We have described the contribution induced by the boundary potential by the symbol $\delta D_p^{\rm c\,(s)}$.

For $u \gg 1$, we have integral equations for ρ and σ as follows (refer to [14]):

$$\rho(k) = \frac{1}{\pi}+{\rm O}\left(\frac{1}{u}\right) \tag{4.6}$$

$$\sigma(\lambda) = \frac{2Q}{\pi}a_1(\lambda)-\int_{-B}^{B}{\rm d}\lambda'\ a_2(\lambda-\lambda')\sigma(\lambda')+{\rm O}\left(\frac{1}{u}\right). \tag{4.7}$$

When we consider the case with $h=0$ (i.e. $B=\infty$), we have

$$\sigma(\lambda) = \frac{n}{2}\frac{1}{\cosh(\pi\lambda/2)}. \tag{4.8}$$

For $0 \leqslant p < 1$ (region 0), the integral equations for $\delta\rho_p$ and $\delta\sigma_p$ take the following forms:

$$\delta\rho_p(k) = \phi_p(k)+{\rm O}\left(\frac{1}{u}\right) \tag{4.9}$$

$$\delta\sigma_p(\lambda) = a_1(\lambda)\int_{-Q}^{Q}{\rm d}k\ \delta\rho_p(k)-\int_{-B}^{B}{\rm d}\lambda'\ a_2(\lambda-\lambda')\,\delta\sigma_p(\lambda')+{\rm O}\left(\frac{1}{u}\right). \tag{4.10}$$

For $1 < p$ (region I), the corresponding integral equations are given by

$$\delta\rho_p(k) = \phi_p(k) + \mathrm{O}\left(\frac{1}{u}\right) \tag{4.11}$$

$$\delta\sigma_p(\lambda) = a_1(\lambda)\left(2 + \int_{-Q}^{Q} \mathrm{d}k\ \delta\rho_p(k)\right) - \int_{-B}^{B} \mathrm{d}\lambda'\ a_2(\lambda - \lambda')\,\delta\sigma_p(\lambda') + \mathrm{O}\left(\frac{1}{u}\right). \tag{4.12}$$

In particular, we have

$$\delta\sigma_p(\lambda) = \begin{cases} \dfrac{\varphi_p(Q)}{2\cosh(\pi\lambda/2)} + \mathrm{O}\left(\dfrac{1}{u}\right) & \text{for } 0 \leqslant p < 1 \\ \dfrac{1+\varphi_p(Q)}{2\cosh(\pi\lambda/2)} + \mathrm{O}\left(\dfrac{1}{u}\right) & \text{for } 0 < p \end{cases} \tag{4.13}$$

for $h = 0$ (i.e. $B = \infty$).

Using the distribution functions of the roots thus obtained, we can arrive at the following results for $h = 0$:

$$\frac{\delta D_p^{\mathrm{c}}}{D_0^{\mathrm{c}}} = \pi\phi_p(n\pi) + \mathrm{O}\left(\frac{1}{u}\right) \tag{4.14}$$

$$\frac{\delta D_p^{\mathrm{s}}}{D_0^{\mathrm{s}}} = \begin{cases} \dfrac{1}{n}\varphi_p(n\pi) + \mathrm{O}\left(\dfrac{1}{u}\right) & 0 \leqslant p < 1 \\ \dfrac{1}{n}(1+\varphi_p(n\pi)) + \mathrm{O}\left(\dfrac{1}{u}\right) & 1 < p. \end{cases} \tag{4.15}$$

Comparing the above results with equations (3.23) and (3.24), we have the following relationships for any p ($\sim\mathrm{O}(u^0)$):

$$\frac{\delta\chi_p^{\mathrm{c}}}{\chi_0^{\mathrm{c}}} = \frac{\delta D_p^{\mathrm{c}}}{D_0^{\mathrm{c}}} \qquad \frac{\delta\chi_p^{\mathrm{s}}}{\chi_0^{\mathrm{s}}} = \frac{\delta D_p^{\mathrm{s}}}{D_0^{\mathrm{s}}} \tag{4.16}$$

ignoring higher-order corrections for a large u. In section 5, we discuss the meaning of these relations.

5. The feasibility of the local Tomonaga–Luttinger liquid

In the present section, we discuss the properties of a local state induced by the boundary potential, using results obtained in sections 3 and 4.

First of all, we recall the local-Fermi-liquid property [19] in the Anderson model from the point of view of Tomonaga–Luttinger liquids [20], as preliminaries. In Tomonaga–Luttinger liquids, the following universal relationships hold:

$$\chi_{\mathrm{c}} = \frac{2K_\rho}{\pi v_{\mathrm{c}}} \qquad \chi_{\mathrm{s}} = \frac{1}{2\pi v_{\mathrm{s}}} \qquad C = \frac{\pi}{3v_{\mathrm{c}}}T + \frac{\pi}{3v_{\mathrm{s}}}T. \tag{5.1}$$

for zero magnetic fields, where $\chi_{\mathrm{c\,(s)}}$ and $v_{\mathrm{c\,(s)}}$ denote the ground-state response function and the Fermi velocity in the charge (spin) sector, respectively. The symbol C denotes the specific heat in a low-temperature region. We describe the Tomonaga–Luttinger parameter by the symbol K_ρ. In the (bulk) conduction electron part of the Anderson model, the relationships in equation (5.1) with $v_{\mathrm{c}} = v_{\mathrm{s}} = v$ hold. Since the bulk part of this model is a free-electron system, the parameter K_ρ takes the value unity. An important property of the Anderson model is that the above relations hold not only for the bulk part but also for the impurity part with the fixed value $K_\rho = 1$. In the impurity part, the parameters v_{c} and v_{s} take the values $v_{\mathrm{c}}^{\mathrm{imp}}$ and $v_{\mathrm{s}}^{\mathrm{imp}}$, respectively, which depend on the strengths of the

interactions in the Anderson model. As was pointed out by Fujimoto, Kawakami and Yang [20], the relationships (5.1) in the impurity part suggest the local-Fermi-liquid properties of the Anderson model.

Since the Hubbard model realizes the Tomonaga–Luttinger liquid (see, e.g., references [13, 14]), the above relations (5.1) hold for the bulk. The Fermi velocities and the Tomonaga–Luttinger parameters depend on the interactions in the Hubbard model. In particular, we have

$$v_{\rm c} = 2\sin(n\pi) \qquad v_{\rm s} = \frac{\pi h_{\rm c}}{4n} \qquad K_\rho = \frac{1}{2} \tag{5.2}$$

for $u \to \infty$ and $h = 0$ [13, 14]. We remark that the parameter K_ρ does not take the value unity, but takes the value of a half due to the strong interactions.

As is well known, the relationships

$$D_0^{\rm c} = \frac{1}{2\pi v_{\rm c}} \qquad D_0^{\rm s} = \frac{1}{2\pi v_{\rm s}} \tag{5.3}$$

hold (see, e.g., reference [18]). By analogy with these relations, we introduce the parameters $v_p^{\rm c}$ and $v_p^{\rm s}$ as follows:

$$\delta D_p^{\rm c} = \frac{1}{2\pi v_p^{\rm c}} \qquad \delta D_p^{\rm s} = \frac{1}{2\pi v_p^{\rm s}}. \tag{5.4}$$

Then, the relations given as equation (4.16) can be rewritten in the following way:

$$\delta\chi_p^{\rm c} = \frac{1}{\pi v_p^{\rm c}} \qquad \delta\chi_p^{\rm s} = \frac{1}{2\pi v_p^{\rm s}}. \tag{5.5}$$

These relationships are similar to those given as equation (5.1) with $K_\rho = 1/2$. If we assume that $v_p^{\rm c}$ and $v_p^{\rm s}$ correspond to Fermi velocities in the local state, the above relations (5.5) seem to suggest that the Tomonaga–Luttinger liquid with $K_\rho = 1/2$ is locally induced by the boundary potential. The similarity between the bulk magnetization equation (3.12) and the induced magnetization equation (3.22) may also suggest that the properties of the local state resemble those in the bulk. We remark that such an induced local state has strong interactions between the electrons (i.e. $K_\rho \neq 1$). In this sense, we may call the state induced by the boundary potential 'the local Tomonaga–Luttinger liquid'. Within our assumptions, the specific heat induced by the boundary potential is expected to take the following form:

$$\delta C_p = \frac{\pi}{3v_p^{\rm c}}T + \frac{\pi}{3v_p^{\rm s}}T \tag{5.6}$$

in a low-temperature region.

Then, we can estimate the Wilson ratio, obtaining

$$R_{\rm W} \equiv \frac{(\delta\chi_p^{\rm s}/\chi_0^{\rm s})}{(\delta C_p/C_0)} = 1 + {\rm O}\left(\frac{1}{u}\right) \tag{5.7}$$

for $h = 0$, where C_0 and $\chi_0^{\rm s}$ denote the specific heat and the susceptibility in the thermodynamic limit, respectively. In this calculation, we have taken it into account that $v_{\rm c} \sim {\rm O}(u^0)$ and $v_{\rm s} \sim {\rm O}(u^{-1})$ for $u \gg 1$. That is, the low-temperature specific heats are evaluated as follows:

$$C_0 = u\left(\frac{\pi}{3uv_{\rm s}}T + {\rm O}\left(\frac{1}{u}\right)\right) \qquad \delta C_p = u\left(\frac{\pi}{3uv_p^{\rm s}}T + {\rm O}\left(\frac{1}{u}\right)\right). \tag{5.8}$$

6. Realization of one-dimensional strongly correlated electron systems with magnetic impurities

In the present paper, we have discussed the properties of the model described by equation (1.1), mainly from a theoretical point of view. However, one-dimensional quantum systems are no longer subjects only of theoretical physics, as is well known. Indeed, various properties of quasi-one-dimensional quantum systems have been observed experimentally; see, e.g., reference [21]. Moreover, one-dimensional quantum systems with magnetic or non-magnetic impurity are also known to be accessible experimentally.

We expect that the Hamiltonian

$$\mathcal{H} = -\sum_{j=1}^{L-1}\sum_{\sigma=\pm}(c_{j\sigma}^{\dagger}c_{j+1\sigma} + c_{j+1\sigma}^{\dagger}c_{j\sigma}) + 4u\sum_{j=1}^{L} n_{j+}n_{j-} + \mu\sum_{j=1}^{L}(n_{j+} + n_{j-}) - \frac{h}{2}\sum_{j=1}^{L}(n_{j+} - n_{j-}) - \ p(n_{1+} + n_{1-}) - p(n_{L+} + n_{L-}) \qquad (0 \leqslant p) \tag{6.1}$$

will lead to an effective theory of a realistic quasi-one-dimensional conductor with magnetic impurities. In particular, for large p, we have the Hubbard open chain with almost localized spins at both ends. In the above model (6.1), the susceptibilities and the specific heat induced by the boundary potential are given as twice the corresponding quantities in the model (1.1).

Indeed, we can dope ions with magnetic moments into a quasi-one-dimensional conductor. Then, we obtain interacting electron chains with impurity spins. Such a system may be described by the Hamiltonian (6.1) with a large p. By observing the specific heat and the susceptibility in quasi-one-dimensional compounds with magnetic impurities, we may be able to obtain local-Tomonaga–Luttinger-liquid properties in such a system.

Experimental and theoretical results for such more realistic systems will be reported in separate papers in the near future.

7. Summary

In the present paper, we have discussed the properties of the model described by the Hamiltonian (1.1) with $u \gg 1$ and $p \sim \mathrm{O}(u^0)$. First, we calculated the compressibility and the susceptibility induced by the boundary potential. Next, we described the quantities in terms of the density of states at the Fermi level. Using the results thus obtained, we discussed the properties of the local state induced by the boundary potential. Our results seem to suggest that the local Tomonaga–Luttinger liquids is realized near the boundary.

It may also be interesting to confirm whether the local Tomonaga–Luttinger liquid can be realized in more realistic situations, e.g. a quasi-one-dimensional conductor with magnetic impurities.

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Appendix A

In this appendix, we give the integral equations for the root densities in the Bethe *ansatz* equation for the model (1.1) in the ground state. The equations have been derived by Bedürftig and Frahm [8]. For detailed derivations, see reference [8].

We describe the distribution functions of the roots ρ_c and ρ_s in the charge and the spin sector, respectively, in the following way:

$$\rho_c(k) = \rho(k) + \frac{1}{L}(\rho_b(k) + \delta\rho_p(k)) + o\left(\frac{1}{L}\right) \tag{A.1}$$

$$\rho_s(\lambda) = \sigma(\lambda) + \frac{1}{L}(\sigma_b(\lambda) + \delta\sigma_p(\lambda)) + o\left(\frac{1}{L}\right). \tag{A.2}$$

Then, the distribution functions of the roots in the bulk ($\rho(k)$ and $\sigma(\lambda)$) are given by the following integral equations:

$$\begin{pmatrix} \rho(k) \\ \sigma(\lambda) \end{pmatrix} = \begin{pmatrix} 1/\pi \\ 0 \end{pmatrix} + \boldsymbol{K} * \begin{pmatrix} \rho(k) \\ \sigma(\lambda) \end{pmatrix}. \tag{A.3}$$

Here, we have introduced an operator $\boldsymbol{K}$ as follows:

$$\boldsymbol{K} * \begin{pmatrix} x_c(k) \\ x_s(\lambda) \end{pmatrix} \equiv \begin{pmatrix} \cos k \displaystyle\int_{-\lambda_0}^{\lambda_0} d\lambda'\ a_u(\sin k - \lambda') x_s(\lambda') \\ \displaystyle\int_{-k_0}^{k_0} dk'\ a_u(\lambda - \sin k') x_c(k') - \int_{-\lambda_0}^{\lambda_0} d\lambda'\ a_{2u}(\lambda - \lambda') x_s(\lambda') \end{pmatrix}. \tag{A.4}$$

For $p = 0$, the boundary contributions to the distribution functions of the roots ($\rho_b(k)$, $\sigma_b(\lambda)$) are given by

$$\begin{pmatrix} \rho_b(k) \\ \sigma_b(\lambda) \end{pmatrix} = \begin{pmatrix} 1/\pi\ -\cos k a_u(\sin k) \\ a_{2u}(\lambda) \end{pmatrix} + \boldsymbol{K} * \begin{pmatrix} \rho_b(k) \\ \sigma_b(\lambda) \end{pmatrix}. \tag{A.5}$$

The distribution functions of the roots induced by the boundary potential are determined by the following integral equations:

$$\begin{pmatrix} \delta\rho_p(k) \\ \delta\sigma_p(\lambda) \end{pmatrix} = \begin{pmatrix} \delta\rho_p^{(0)}(k) \\ \delta\sigma_p^{(0)}(\lambda) \end{pmatrix} + \boldsymbol{K} * \begin{pmatrix} \delta\rho_p(k) \\ \delta\sigma_p(\lambda) \end{pmatrix} \tag{A.6}$$

with

$$\delta\rho_p^{(0)}(k) \equiv \phi_p(k) + \begin{cases} 0 & \text{for regions 0 and I} \\ \cos k(a_t(\sin k) + a_{2u-t}(\sin k)) & \text{for region II} \\ \cos k(a_t(\sin k) - a_{t-2u}(\sin k)) & \text{for region III} \end{cases} \tag{A.7}$$

$$\delta\sigma_p^{(0)}(\lambda) \equiv \begin{cases} 0 & \text{for regions 0 and III} \\ a_{u-t}(\lambda) + a_{u+t}(\lambda) & \text{for region I} \\ -a_{t-u}(\lambda) - a_{3t-u}(\lambda) & \text{for region II.} \end{cases} \tag{A.8}$$

Using the distribution functions of the roots thus determined, we can describe the ground-state energy as follows:

$$\frac{E}{L} = \frac{1}{2}\int_{-k_0}^{k_0} dk\ \varepsilon_c^{(0)}(k)\rho_c(k) + \frac{1}{2}\int_{-\lambda_0}^{\lambda_0} d\lambda\ \varepsilon_s^{(0)}(\lambda)\rho_s(\lambda) + \frac{1}{L}\left(-\frac{1}{2}(\varepsilon_c^{(0)}(0) + \varepsilon_s^{(0)}(0)) + E_p\right) + o\left(\frac{1}{L}\right) \tag{A.9}$$

with

$$E_p = \begin{cases} 0 & \text{for region 0} \\ E_1 & \text{for region I} \\ E_1 + h & \text{for region II} \\ E_1 + E_2 + h & \text{for region III.} \end{cases} \tag{A.10}$$

Here, we have introduced parameters as follows:

$$\varepsilon_{\mathrm{c}}^{(0)}(k) \equiv \mu - \frac{h}{2} - 2\cos k \qquad \varepsilon_{\mathrm{s}}^{(0)}(\lambda) \equiv h \tag{A.11}$$

and

$$E_1 \equiv -2t + \mu - \frac{h}{2} \qquad E_2 \equiv -2\sqrt{1 + (t - 2u)^2} + \mu - \frac{h}{2} \tag{A.12}$$

with $t \equiv \frac{1}{2}(p - p^{-1})$.

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