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Boundary scattering matrices in the Hubbard model with boundary fields

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Abstract. Elementary excitations in the one-dimensional Hubbard model with boundary fields are discussed. Boundary scattering matrices for the excitations of the charge and spin sectors are evaluated. Both the repulsive and the attractive Hubbard models at half-filling and without a magnetic field are studied.

1. Introduction

In the present paper, we study the elementary excitations of the one-dimensional Hubbard model with boundary fields, which is described by

$$\mathcal{H} = -\sum_{j=1}^{L-1}\sum_{\sigma=\pm}\left(c_{j\sigma}^{\dagger}c_{j+1\sigma} + c_{j+1\sigma}^{\dagger}c_{j\sigma}\right) + 4u\sum_{j=1}^{L}\left(n_{j+} - \tfrac{1}{2}\right)\left(n_{j-} - \tfrac{1}{2}\right)$$
$$+ q_{1+}n_{1+} + q_{1-}n_{1-} + q_{L+}n_{L+} + q_{L-}n_{L-}. \tag{1.1}$$

Here the symbol $c_{j\sigma}$ ($c_{j\sigma}^{\dagger}$) denotes the annihilation (creation) operator of the electron with the spin σ at the site j, and $n_{j\sigma}$ is defined by $n_{j\sigma} = c_{j\sigma}^{\dagger}c_{j\sigma}$. In the present paper, we take an even integer as L.

The purpose of the present paper is to derive the boundary scattering matrices for the quasiparticles corresponding to the charge and the spin excitations of the Hubbard model with boundary fields (1.1). Essler and Korepin [1] and Andrei [2] studied scattering matrices in the Hubbard model under a *periodic* boundary condition. They determined the two-particle scattering matrices in the *bulk* [1, 2]. In the present study, we determine the scattering matrices of the quasiparticles at the *boundary*. In our previous study [3], we have discussed the elementary excitations of the Hubbard model with *free* boundaries, which is described by the Hamiltonian (1.1) with $q_{1\pm} = q_{L\pm} = 0$. We have already obtained the scattering matrices of the quasiparticles at a *free* boundary, as a part of our results in [3].

In order to derive the scattering matrices exactly, we need the Bethe-ansatz equations for the Hubbard model with boundary fields. For the following four kinds of boundary fields, the Bethe-ansatz equation of the present model (1.1) has been derived.

Case A: $q_{1\pm} = q_1$ and $q_{L\pm} = q_L$ (aa type) [4],
Case B: $q_{1\pm} = \pm q_1$ and $q_{L\pm} = \pm q_L$ (bb type) [5–7],

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Case C: $q_{1\pm} = \pm q_1$ and $q_{L\pm} = q_L$ (ba type) [5, 6],
Case D: $q_{1\pm} = q_1$ and $q_{L\pm} = \pm q_L$ (ab type) [5, 6].

Here the a-type (b-type) boundary field corresponds to the chemical potential (the magnetic field) at a boundary site. (The Bethe-ansatz equation under the free boundary condition, i.e. $q_{1\pm} = q_{L\pm} = 0$, has been derived by Schulz [8].) The Bethe-ansatz equation for each case takes the following form [4–7]:

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} Z(k_j; q_1, q_L) = \prod_{\beta=1}^{M} \frac{\sin k_j - \lambda_\beta + \mathrm{i}u}{\sin k_j - \lambda_\beta - \mathrm{i}u} \frac{\sin k_j + \lambda_\beta + \mathrm{i}u}{\sin k_j + \lambda_\beta - \mathrm{i}u} \tag{1.2}$$

$$\prod_{l=1}^{N} \frac{\lambda_\alpha - \sin k_l + \mathrm{i}u}{\lambda_\alpha - \sin k_l - \mathrm{i}u} \frac{\lambda_\alpha + \sin k_l + \mathrm{i}u}{\lambda_\alpha + \sin k_l - \mathrm{i}u} = Y(\lambda_\alpha; q_1, q_L) \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{\lambda_\alpha - \lambda_\beta + 2\mathrm{i}u}{\lambda_\alpha - \lambda_\beta - 2\mathrm{i}u} \frac{\lambda_\alpha + \lambda_\beta + 2\mathrm{i}u}{\lambda_\alpha + \lambda_\beta - 2\mathrm{i}u}$$

$$j = 1, \ldots, N \quad \alpha = 1, \ldots, M \tag{1.3}$$

where N (M) denotes the total number of the electrons (the number of the electrons with down spins). Here we have defined

$$Z(k; q_1, q_L) \equiv \zeta(k; q_1)\zeta(k; q_L) \qquad \text{for cases } A,\ B,\ C \text{ and } D \tag{1.4}$$

$$Y(\lambda; q_1, q_L) \equiv \begin{cases} 1 & \text{for case } A \\ \eta(\lambda; q_1)\eta(\lambda; q_L) & \text{for case } B \\ \eta(\lambda; q_1) & \text{for case } C \\ \eta(\lambda; q_L) & \text{for case } D \end{cases} \tag{1.5}$$

with

$$\zeta(k; q) \equiv \frac{1 + q\mathrm{e}^{-\mathrm{i}k}}{1 + q\mathrm{e}^{\mathrm{i}k}} \qquad \eta(\lambda; q) \equiv -\frac{\lambda + \mathrm{i}\left(u - \frac{1}{2}(q^{-1} - q)\right)}{\lambda - \mathrm{i}\left(u - \frac{1}{2}(q^{-1} - q)\right)}. \tag{1.6}$$

Then, the energy of the present model is given by

$$E = \sum_{j=1}^{N} \left(-2\cos k_j - 2u\right) + uL. \tag{1.7}$$

We can restrict the solutions of the above Bethe-ansatz equations as follows:

$$0 \leqslant \mathrm{Re}(k_j) \leqslant \pi \quad k_j \neq 0, \pi \qquad \text{and} \qquad \mathrm{Re}(\lambda_\alpha) \geqslant 0 \quad \lambda_\alpha \neq 0, \infty \tag{1.8}$$

so that we obtain independent Bethe states. We refer the reader to the Bethe-ansatz wavefunction in the present model [4, 8]. See also, e.g., [9, 10]. (In order to derive the boundary scattering matrices for the a-type and b-type boundary fields we only have to consider two cases, i.e. case A (aa type) and case B (bb type), since the contributions from the both ends are independent of each other.)

The *periodic* Hubbard chain is invariant under an $SO(4) = SU(2) \times SU(2)/Z_2$ transformation [11]. Consequently, the Hubbard chain with the periodic boundary condition has four elementary excitations (i.e. quasiparticles), which form the fundamental representation of $SU(2) \times SU(2)$, accurately $SO(4)$ [1]. A couple of these elementary excitations carries spin but no charge, and the other couple carries charge but no spin. The *bulk terms* in the *open* Hubbard chain with boundary fields (1.1) are also $SO(4)$

$= SU(2) \times SU(2)/Z_2$ invariant. Indeed, if we neglect the boundary terms or the boundary fields vanish in (1.1), all the following six generators:

$$\mathcal{S}^+ = \sum_{j=1}^{L} c_{j+}^\dagger c_{j-} \qquad \mathcal{S}^- = \sum_{j=1}^{L} c_{j-}^\dagger c_{j+} \qquad \mathcal{S}^z = \frac{1}{2}\sum_{j=1}^{L}\left(n_{j+} - n_{j-}\right) \tag{1.9}$$

$$\mathcal{T}^+ = \sum_{j=1}^{L}(-1)^j c_{j+} c_{j-} \qquad \mathcal{T}^- = \sum_{j=1}^{L}(-1)^j c_{j-}^\dagger c_{j+}^\dagger \qquad \mathcal{T}^z = -\frac{1}{2}\sum_{j=1}^{L}\left(n_{j+} + n_{j-} - 1\right) \tag{1.10}$$

commute with the Hamiltonian (1.1). The Z_2 quotient corresponds to the fact that operator $\mathcal{S}^z + \mathcal{T}^z$ has only integer eigenvalues as L is even. The operators $\{\mathcal{S}^+, \mathcal{S}^-, \mathcal{S}^z\}$ and $\{\mathcal{T}^+, \mathcal{T}^-, \mathcal{T}^z\}$ correspond to the $SU(2)$ symmetry in the spin degree of freedom and that in the charge degree of freedom, respectively. (In the present paper, we specify the total $SU(2)$ spin (charge) by the quantum number S (T) and describe the z-component $\mathcal{S}^z$ $(\mathcal{T}^z)$ by the quantum number S^z (T^z).) Since the properties of the elementary excitations in the bulk do not depend on boundary conditions, the behaviours of the quasiparticles in the present model (1.1) are already known except for the boundary scatterings. The local violation of $SO(4)$ symmetry due to the boundary fields is expected to influence the scattering at the boundary, as with other models, e.g., the Heisenberg model [9, 10] and the supersymmetric t–J model [12]. Here we remark that the a-type boundary breaks the charge $SU(2)$ symmetry (generated by $\{\mathcal{T}^+, \mathcal{T}^-, \mathcal{T}^z\}$) and the b-type boundary breaks the spin $SU(2)$ symmetry (generated by $\{\mathcal{S}^+, \mathcal{S}^-, \mathcal{S}^z\}$).

The way to determine the boundary scattering matrices has been established through recent works [9, 10, 18]. Ghoshal and Zamolodchikov [18] generalized the bootstrap approach for determining the bulk scattering matrix [17] to derive the boundary scattering matrix of the boundary sine-Gordon model. Fendley and Saleur [9] and Grisaru *et al* [10] proposed alternative approaches to determine the boundary scattering matrix for the Heisenberg open chain directly from the Bethe-ansatz equation. In the present paper, we use the method by Grisaru *et al* [10]. Their method [10] is based on the following quantization condition for factorized scattering of two particles with repidities λ_1 and λ_2 on a line of length $\bar{L}$:

$$\exp\left(\mathrm{i}p(\lambda_1)2\bar{L}\right) S_{12}(\lambda_1 - \lambda_2) K_1^{\mathrm{L}}(\lambda_1) S_{12}(\lambda_1 + \lambda_2) K_1^{\mathrm{R}}(\lambda_1) = 1. \tag{1.11}$$

This condition comes from the requirement that the wavefunction should vanish at the both ends of the line [9, 10]. Here we describe the physical momentum of a quasiparticle with a rapidity λ by the symbol $p(\lambda)$. The symbol $S_{12}(\lambda)$ denotes the bulk scattering matrix of the particles labelled by '1' and '2'. The symbol $K_1^{\mathrm{L(R)}}(\lambda)$ denotes the boundary scattering matrix describing the scattering of a boundary at the left (right) end. (For detailed discussions on the quantization condition, see [10].)

By using the above quantization condition [10], we determine the boundary scattering matrices in the charge sector and the spin sector for each of the following four cases:

- a-type boundary field in the repulsive Hubbard model (section 2),
- b-type boundary field in the repulsive Hubbard model (section 2),
- a-type boundary field in the attractive Hubbard model (section 3),
- b-type boundary field in the attractive Hubbard model (section 3).

Recently, another author [13] calculated boundary scattering matrices in the repulsive Hubbard model with the a-type boundary field. He remarked [13] that quasiparticle spectra of the repulsive and the attractive Hubbard models are related by an interchange of the spin and charge degrees of freedom [13], although he did not derive the scattering matrices in the attractive Hubbard model explicitly. In the present paper, we derive the boundary scattering matrices for the above four cases explicitly.

Since we need the information about the two-body scattering in the bulk [1, 2] in deriving the boundary scattering matrices, we briefly review the known results about the properties of the quasiparticles in the Hubbard chain and their two-body scattering matrix in subsections 2.1 and 3.1. In our calculations, we also have to adopt the string hypothesis [14] for the solutions of the Bethe-ansatz equation. In subsections 2.2 and 3.2, we briefly explain the string forms of the solutions for the Hubbard chain, as preliminaries. We determine the boundary scattering matrices for $u > 0$ in subsections 2.3 (charge sector) and 2.4 (spin sector). For $u < 0$, we obtain the matrices describing the boundary scattering in subsection 3.3 (spin sector) and 3.4 (charge sector).

2. Repulsive Hubbard open chain

2.1. Review of the bulk scattering matrix

In this subsection, we briefly review the two-body scattering matrix [1, 2] of the elementary excitations in the (infinitely long) periodic Hubbard chain with the $SO(4)$ symmetry for $u > 0$. (For detailed explanations, see, e.g., [1, 2] and references therein.)

The repulsive Hubbard model has four elementary excitations, which forms fundamental representation of $SU(2)_{\text{spin}} \times SU(2)_{\text{charge}}$ [1, 2]. Two of them carry spin but no charge to form a doublet of the spin $SU(2)$. Each of them is a singlet with respect to the charge $SU(2)$. Namely, their quantum numbers can be described as $S = \frac{1}{2}$, $S^z = \pm\frac{1}{2}$ and $T = 0$. These two excitations (quasiparticles) are called spinons, and have the momentum $p_{\text{s}}(\lambda)$ and the energy $\varepsilon_{\text{s}}(\lambda)$:

$$p_{\text{s}}(\lambda) = \frac{\pi}{2} - \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_0(\omega)\sin(\omega\lambda)}{\cosh(\omega u)} \tag{2.1}$$

$$\varepsilon_{\text{s}}(\lambda) = 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)\cos(\omega\lambda)}{\cosh(\omega u)}. \tag{2.2}$$

Here the symbol $J_n(\omega)$ denotes the Bessel function. The other two elementary excitations carry charge but no spin to form a doublet with respect to the charge $SU(2)$ and a singlet of the spin $SU(2)$. Namely, they have the quantum numbers $T = \frac{1}{2}$, $T^z = \pm\frac{1}{2}$ and $S = 0$. These two excitations (quasiparticles) are called holon for $T^z = \frac{1}{2}$ and antiholon for $T^z = -\frac{1}{2}$. The holon (antiholon) has the momentum $p_{\text{c}}^{\text{h}}(k)$ ($p_{\text{c}}^{\text{ah}}(k)$) and the energy $\varepsilon_{\text{c}}^{\text{h}}(k)$ ($\varepsilon_{\text{c}}^{\text{ah}}(k)$) described by

$$p_{\text{c}}^{\text{h}}(k) = \frac{\pi}{2} - k - \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_0(\omega)\sin(\omega\sin k)\mathrm{e}^{-\omega u}}{\cosh(\omega u)} = \pi + p_{\text{c}}^{\text{ah}}(k) \tag{2.3}$$

$$\varepsilon_{\text{c}}^{\text{h}}(k) = 2u + 2\cos k + 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)\cos(\omega\sin k)\,\mathrm{e}^{-\omega u}}{\cosh(\omega u)} = \varepsilon_{\text{c}}^{\text{ah}}(k). \tag{2.4}$$

The two-body scattering matrix of these elementary excitations is 16-dimensional and block-diagonal, which is described by

$$S = \begin{pmatrix} S_{\text{ss}}(\mu_1) & 0 & 0 & 0 \\ 0 & S_{\text{sc}}(\mu_2) & 0 & 0 \\ 0 & 0 & S_{\text{cs}}(\mu_3) & 0 \\ 0 & 0 & 0 & S_{\text{cc}}(\mu_4) \end{pmatrix}. \tag{2.5}$$

At first, the matrix S_{ss} describes scattering of two spinons (with rapidities λ_1 and λ_2), and is of the form

$$S_{ss}(\mu) = -\frac{\Gamma\left(\frac{1}{2}+\frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1-\frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2}-\frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1+\frac{1}{2}\mathrm{i}\mu\right)}\left(\frac{\mu\mathcal{I}+\mathrm{i}\mathcal{P}}{\mu+\mathrm{i}}\right) \qquad \mu = \frac{\lambda_1-\lambda_2}{2u} \quad (>0) \tag{2.6}$$

where $\mathcal{I}$ and $\mathcal{P}$ denote the 4×4 identity and permutation matrices, respectively. The four-dimensional space of S_{ss} corresponds to the four degenerate states with two spinons, i.e. the triplet ($S=1$) and the singlet ($S=0$) states. Next, the scattering matrix S_{cc} for two holons/antiholons (with rapidities k_1 and k_2) is given by

$$S_{cc}(\mu) = \frac{\Gamma\left(\frac{1}{2}-\frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1+\frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2}+\frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1-\frac{1}{2}\mathrm{i}\mu\right)}\left(\frac{\mu\mathcal{I}-\mathrm{i}\mathcal{P}}{\mu-\mathrm{i}}\right) \qquad \mu = \frac{\sin k_1-\sin k_2}{2u} \quad (>0). \tag{2.7}$$

This matrix S_{cc} is described in the space spanned by the four degenerate states with two holons/antiholons, i.e. the triplet ($T=1$) and the singlet ($T=0$) states. The scattering of one spinon and one holon/antiholon is described by

$$S_{sc}(\mu) = -\mathrm{i}\frac{1+\mathrm{i}\exp(\pi\mu)}{1-\mathrm{i}\exp(\pi\mu)}\mathcal{I} \qquad \mu = \frac{\lambda-\sin k}{2u} \quad (>0) \tag{2.8}$$

$$S_{cs}(\mu) = -\mathrm{i}\frac{1+\mathrm{i}\exp(\pi\mu)}{1-\mathrm{i}\exp(\pi\mu)}\mathcal{I} \qquad \mu = \frac{\sin k-\lambda}{2u} \quad (>0). \tag{2.9}$$

2.2. String hypothesis

In deriving the boundary scattering matrices in subsections 2.3 and 2.4, we shall assume that the string hypothesis [14] holds in the solutions of the Bethe-ansatz equation for the Hubbard model with boundaries similarly to the periodic-boundary case. (Also in other models, e.g., the Heisenberg model [9, 10] and the supersymmetric t–J model [12], the solutions of the Bethe-ansatz equations for the open chain are expected to take the same string forms as those for the periodic chain.) In this subsection, we briefly explain the string forms [14] of the solutions in the Bethe-ansatz equation for the repulsive Hubbard chain.

We assume that the solutions of the Bethe-ansatz equation for the repulsive Hubbard chain take the following string forms [14].

(1) λ-strings: n λ_α's combine into a string-type configuration to take the form

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \mathrm{i}(n+1-2j)u \qquad j=1,\ldots,n \quad \alpha=1,\ldots,M_n$$

with a real number λ_α^n, apart from a correction of order $\mathrm{e}^{-\delta L}$. Here the symbol δ denotes a positive number.

(2) k–λ-strings: $2n$ k_j's and n λ_α's combine into another string-type configuration and take the following forms to $\mathrm{O}(\mathrm{e}^{-\delta L})$:

$$\lambda'^{n,j}_\alpha = \lambda'^n_\alpha + \mathrm{i}(n+1-2j)u \qquad j=1,\ldots,n \quad \alpha=1,\ldots,M'_n$$

with a real number λ'^n_α, and

$$k_\alpha^1 = \pi - \sin^{-1}(\lambda'^n_\alpha + \mathrm{i}nu)$$

$$k_\alpha^2 = \sin^{-1}(\lambda'^n_\alpha + \mathrm{i}(n-2)u) \qquad k_\alpha^3 = \pi - k_\alpha^2$$

$$k_\alpha^4 = \sin^{-1}(\lambda'^n_\alpha + \mathrm{i}(n-4)u) \qquad k_\alpha^5 = \pi - k_\alpha^4$$

$$\vdots$$

$$k_\alpha^{2n-2} = \sin^{-1}(\lambda'^{n}_{\alpha} - \mathrm{i}(n-2)u) \qquad k_\alpha^{2n-1} = \pi - k_\alpha^{2n-2}$$

$$k_\alpha^{2n} = \pi - \sin^{-1}(\lambda'^{n}_{\alpha} - \mathrm{i}nu).$$

(3) Real k_j, which do not form the above string-type configurations. (Hereafter, we describe only this type of real element in $\{k_j\}$ by the symbol k_j.)

If we introduce the number M' by $M' = \sum_{n=1}^{\infty} nM'_n$, the number of real k_j's is equal to $N - 2M'$. We also find that the relationship $M = \sum_{n=1}^{\infty} nM_n + \sum_{n=1}^{\infty} nM'_n$ holds.

The ground state of the present model (1.1) with $u > 0$ corresponds to the case with $N = L$, $M_1 = L/2$, $M_n = 0$ ($n \geqslant 2$) and $M'_n = 0$ ($n \geqslant 1$).

2.3. Charge sector

In this subsection, we derive the boundary scattering matrices for the elementary excitation of the charge sector for $u > 0$.

For this purpose, we take it into account that the quantization condition for factorized scattering of two particles holds [9, 10]. We can describe the quantization condition for factorized scattering of two particles with rapidities k_1 and k_2 on a line of length $\overline{L}$, as follows:

$$\exp(\mathrm{i}p_{\mathrm{c}}(k_1)2\overline{L})S_{\mathrm{cc}}(\theta_1 - \theta_2)K_{\mathrm{c}}(k_1; q_1)S_{\mathrm{cc}}(\theta_1 + \theta_2)K_{\mathrm{c}}(k_1; q_L) = 1 \tag{2.10}$$

with $\theta_j \equiv \sin k_j/(2u)$ for $j = 1, 2$. The quantity $p_{\mathrm{c}}(k)$ takes the holon momentum $p_{\mathrm{c}}^{\mathrm{h}}(k)$ (the antiholon momentum $p_{\mathrm{c}}^{\mathrm{ah}}(k)$) for $T^z = \frac{1}{2}$ ($T^z = -\frac{1}{2}$). For the triplet state ($T = 1$), the bulk scattering matrix S_{cc} is of the form [1]

$$S_{\mathrm{cc}}(\mu) = \exp\left(\mathrm{i}\psi_{\mathrm{cc}}(\mu)\right) \qquad \psi_{\mathrm{cc}}(\mu) = \frac{1}{\mathrm{i}}\ln\left(\frac{\Gamma\left(\frac{1}{2} - \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 + \frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2} + \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 - \frac{1}{2}\mathrm{i}\mu\right)}\right). \tag{2.11}$$

The $U(1)$ symmetry of the boundary terms in eq.(1.1) implies that the boundary scattering matrix $K_{\mathrm{c}}(k; q)$ takes the following form:

$$K_{\mathrm{c}}(k; q) = \begin{pmatrix} \exp\left(\mathrm{i}\phi_{\mathrm{c}}^{+}(k; q)\right) & 0 \\ 0 & \exp\left(\mathrm{i}\phi_{\mathrm{c}}^{-}(k; q)\right) \end{pmatrix}. \tag{2.12}$$

Here this matrix is represented in the two-dimensional space spanned by the states with $T^z = \pm\frac{1}{2}$. Then, the quantization condition yields the following relationships:

$$2\overline{L}p_{\mathrm{c}}^{\mathrm{h}}(k_1) + \psi_{\mathrm{cc}}(\theta_1 - \theta_2) + \phi_{\mathrm{c}}^{+}(k_1; q_1) + \psi_{\mathrm{cc}}(\theta_1 + \theta_2) + \phi_{\mathrm{c}}^{+}(k_1; q_L) = 0 \pmod{2\pi} \tag{2.13}$$

for the $T^z = 1$ state, and

$$2\overline{L}p_{\mathrm{c}}^{\mathrm{ah}}(k_1) + \psi_{\mathrm{cc}}(\theta_1 - \theta_2) + \phi_{\mathrm{c}}^{-}(k_1; q_1) + \psi_{\mathrm{cc}}(\theta_1 + \theta_2) + \phi_{\mathrm{c}}^{-}(k_1; q_L) = 0 \pmod{2\pi} \tag{2.14}$$

for the $T^z = -1$ state. Here we should take $L + 1$ as $\overline{L}$ for models defined on a chain with L sites [3]. What we have to do here is to determine the phase shifts $\phi_{\mathrm{c}}^{\pm}(k; q)$.

Within the string hypothesis, the state with $T^z = 1$ is characterized by two holes in the sea of real roots of $\{k_j\}$ and no holes in the sea of real $\{\lambda_\alpha\}$. Namely, this state corresponds to the case with $N = L - 2$, $M_1 = L/2 - 1$, $M_n = 0$ ($n \geqslant 2$) and $M'_n = 0$ ($n \geqslant 1$). Then, we can rewrite the Bethe-ansatz equations in the following forms:

$$\frac{I_j}{L} = z_{\mathrm{c}}(k_j) \qquad \text{and} \qquad \frac{J_\alpha}{L} = z_{\mathrm{s}}(\lambda_\alpha) \tag{2.15}$$

$$2\pi z_{\rm c}(k) \equiv 2\left(1+\frac{1}{L}\right)k - \frac{\rm i}{L}\ln Z(k) + \frac{1}{L}\sum_{\beta=1}^{L/2-1}\left\{\theta\left(\frac{\sin k-\lambda_\beta}{u}\right)+\theta\left(\frac{\sin k+\lambda_\beta}{u}\right)\right\} \tag{2.16}$$

$$\begin{aligned}2\pi z_{\rm s}(\lambda) \equiv{}& \frac{1}{L}\theta\left(\frac{\lambda}{u}\right) - \frac{\rm i}{L}\ln Y(\lambda) + \frac{1}{L}\sum_{l=1}^{L}\left\{\theta\left(\frac{\lambda-\sin k_l}{u}\right)+\theta\left(\frac{\lambda+\sin k_l}{u}\right)\right\}\\ &-\frac{1}{L}\sum_{j=1}^{2}\left\{\theta\left(\frac{\lambda-\sin k_j^{\rm h}}{u}\right)+\theta\left(\frac{\lambda+\sin k_j^{\rm h}}{u}\right)\right\}\\ &-\frac{1}{L}\sum_{\beta=1}^{L/2-1}\left\{\theta\left(\frac{\lambda-\lambda_\beta}{2u}\right)+\theta\left(\frac{\lambda+\lambda_\beta}{2u}\right)\right\}\end{aligned} \tag{2.17}$$

with $\theta(x) = 2\tan^{-1}x$. Here $\{I_j\}$ $(j = 1,\ldots,L)$ and $\{J_\alpha\}$ $(\alpha = 1,\ldots,L/2-1)$ take positive integer values. Two of $\{I_j\}$ correspond to the holes with the rapidities $k_1^{\rm h}$ and $k_2^{\rm h}$. By neglecting contributions smaller than $1/L$, we have

$$\begin{aligned}2\pi z_{\rm c}(k) ={}& -2\left(1+\frac{1}{L}\right)\left(p_{\rm c}^{\rm h}(k)-p_{\rm c}^{\rm h}(0)\right) - \frac{1}{L}\left(\mathcal{B}_{\rm c}(k;q_1)+\mathcal{B}_{\rm c}(k;q_L)\right) - \frac{1}{L}\Psi(\sin k)\\ &-\frac{1}{L}\left\{\sum_{j=1}^{2}\left(\Phi(\sin k-\sin k_j^{\rm h})+\Phi(\sin k+\sin k_j^{\rm h})\right)+\Phi(\sin k)\right\}\end{aligned} \tag{2.18}$$

where

$$\Psi(\lambda) = {\rm i}\int_{-\infty}^{\infty}\frac{{\rm e}^{-{\rm i}\omega\lambda}}{2\cosh u\omega}\frac{{\rm d}\omega}{\omega} \qquad \Phi(\lambda) = {\rm i}\int_{-\infty}^{\infty}\frac{{\rm e}^{-|u\omega|}{\rm e}^{-{\rm i}\omega\lambda}}{2\cosh u\omega}\frac{{\rm d}\omega}{\omega} \tag{2.19}$$

$$\mathcal{B}_{\rm c}(k;q) = \frac{1}{\rm i}\ln\frac{1+q{\rm e}^{{\rm i}k}}{1+q{\rm e}^{-{\rm i}k}} + \frac{1}{\rm i}\int_{-\infty}^{\infty}\frac{{\rm d}\omega}{\omega}\frac{{\rm e}^{-{\rm i}\omega\sin k}}{2\cosh u\omega}\tilde{\mathcal{A}}_{\rm R}(\omega;q). \tag{2.20}$$

Here the function $\tilde{\mathcal{A}}_{\rm R}$ is given by $\tilde{\mathcal{A}}_{\rm R}(\omega;q) = \int_{-\infty}^{\infty}{\rm d}\lambda\,\mathcal{A}_{\rm R}(\lambda;q){\rm e}^{{\rm i}\omega\lambda}$, where

$$\mathcal{A}_{\rm R}(\lambda;q) = \begin{cases}\displaystyle\int_{-\pi}^{\pi}{\rm d}k\ a_1(\lambda-\sin k)\mathcal{A}_0(k;q) & \text{for type } a\\ \displaystyle\int_{-\pi}^{\pi}{\rm d}k\ a_1(\lambda-\sin k)\mathcal{A}_0(k;q)+\mathcal{A}_1(\lambda;q) & \text{for type } b\end{cases} \tag{2.21}$$

$$\begin{aligned}a_\nu(\lambda) &= \frac{1}{\pi}\frac{\nu|u|}{\lambda^2+(\nu u)^2}\\ \mathcal{A}_0(k;q) &= \frac{1}{2\pi{\rm i}}\frac{\rm d}{{\rm d}k}\ln\zeta(k;q)\\ \mathcal{A}_1(\lambda;q) &= \frac{1}{2\pi{\rm i}}\frac{\rm d}{{\rm d}\lambda}\ln\eta(\lambda;q).\end{aligned} \tag{2.22}$$

When we need to express the fact that the function $\mathcal{A}_{\rm R}(\lambda;q)$ depends on the parameter u and the type of boundary fields (a or b), we describe this function as $\mathcal{A}_{\rm R}^x(\lambda;q|u)$ with $x = a, b$. In deriving equation (2.18), we have neglected higher-order corrections to rewrite the summations in (2.16), (2.17) as integrals. Then, we have made the assumption that the contributions due to the shift of integration boundaries are of higher order in $1/L$, as in the cases of other models [9, 10, 12]. Using the functions z_{c} and z_{s} thus obtained, we have

$$-2\pi z_{\mathrm{c}}(k_1)L = 2(L+1)\left(p_{\mathrm{c}}^{\mathrm{h}}(k_1) - p_{\mathrm{c}}^{\mathrm{h}}(0)\right) + \Phi(\sin k_1 - \sin k_2) + \Phi(\sin k_1 + \sin k_2)$$
$$+\Psi(\sin k_1) + \Phi(\sin k_1) + \Phi(2\sin k_1) + \mathcal{B}_{\mathrm{c}}(k_1; q_1) + \mathcal{B}_{\mathrm{c}}(k_1; q_L) \qquad (2.23)$$

where we have abbreviated k_j^{h} by k_j. Here the equality

$$2\pi z_{\mathrm{c}}(k_1)L = 0 \pmod{2\pi} \qquad (2.24)$$

holds since evaluation for Lz_{c} at a root of the Bethe-ansatz equations yields an integer by definition. Comparing equations (2.23), (2.24) with (2.13), we can recognize the relationship

$$\phi_{\mathrm{c}}^{+}(k;q) = \phi_{\mathrm{c}}^{(0)}(k) + \delta_{\mathrm{c}}^{+}(k;q) \qquad (2.25)$$

$$\phi_{\mathrm{c}}^{(0)}(k) = \tfrac{1}{2}\left(\Psi(\sin k) + \Phi(\sin k) + \Phi(2\sin k)\right) \qquad \delta_{\mathrm{c}}^{+}(k;q) = \mathcal{B}_{\mathrm{c}}(k;q) \qquad (2.26)$$

holds apart from rapidity-independent constants. We have already derived $\phi_{\mathrm{c}}^{(0)}$ using the Bethe-ansatz equation for the Hubbard model with free boundaries [3]. We can rewrite the phase shifts $\phi_{\mathrm{c}}^{(0)}$ and δ_{c}^{+} to have

$$\phi_{\mathrm{c}}^{(0)}(k) = \frac{1}{\mathrm{i}}\ln\left(\frac{\Gamma\left(1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{4}-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{4}+\frac{1}{2}\mathrm{i}\theta\right)}\right) \qquad \theta = \frac{\sin k}{2u} \qquad (2.27)$$

$$\delta_{\mathrm{c}}^{+}(k;q) = \begin{cases} \dfrac{1}{\mathrm{i}}\ln\dfrac{1+q\mathrm{e}^{\mathrm{i}k}}{1+q\mathrm{e}^{-\mathrm{i}k}} + \Theta_{\mathrm{c}}(k;q) & \text{for type } a \\ \dfrac{1}{\mathrm{i}}\ln\left(\dfrac{1+q\mathrm{e}^{\mathrm{i}k}}{1+q\mathrm{e}^{-\mathrm{i}k}}\dfrac{\Gamma\left(\frac{1}{2}\xi+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)+\frac{1}{2}\mathrm{i}\theta\right)}\right) & \\ \qquad + \Theta_{\mathrm{c}}(k;q) & \text{for type } b \end{cases} \qquad (2.28)$$

with

$$\Theta_{\mathrm{c}}(k;q) = \frac{1}{\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\mathrm{e}^{-\mathrm{i}\omega\sin k}\frac{\mathrm{e}^{-u|\omega|}}{2\cosh u\omega}\left(2\sum_{j=1}^{\infty}q^{2j}J_{2j}(\omega)\right). \qquad (2.29)$$

In the present paper, we define the parameter ξ to be $\xi \equiv (q^{-1}-q)/(4|u|)$ for $u > 0$ and $u < 0$. In calculating the phase shift for the type-b boundary field, we have constrained ourselves to the region $1 > q > 0$ and $\xi > \frac{1}{2}$.

Next, we discuss the case with $T^z = -1$. We consider the following canonical transformation:

$$c_{j+} \longrightarrow (-1)^j c_{j-}^{\dagger} \qquad \text{and} \qquad c_{j-} \longrightarrow (-1)^j c_{j+}^{\dagger} \qquad (2.30)$$

which keeps the Hamiltonian (1.1) without boundary fields invariant. The present transformation does not change the type-b boundary field, but changes the sign of the type-a boundary field. We also remark that the operators $\sum_{\alpha=x,y,z}\mathcal{S}^{\alpha}\mathcal{S}^{\alpha}$, $\mathcal{S}^z$ and $\sum_{\alpha=x,y,z}\mathcal{T}^{\alpha}\mathcal{T}^{\alpha}$ are invariant, and $\mathcal{T}^z$ changes into $-\mathcal{T}^z$, under the transformation. Therefore, we can obtain the state with $T^z = -1$ of the Hubbard model (1.1) as that with $T^z = 1$ of the model with the type-a boundary field reversed. After similar calculations to the previous case, we arrive at the following results:

$$\phi_{\mathrm{c}}^{-}(k;q) = \phi_{\mathrm{c}}^{(0)}(k) + \delta_{\mathrm{c}}^{-}(k;q) \qquad \delta_{\mathrm{c}}^{-}(k;q) = \mathcal{B}_{\mathrm{c}}(k;-q) \qquad (2.31)$$

apart from rapidity-independent constants. The above equation holds for both of the type-a and the type-b boundary fields, since the function $\mathcal{B}_{\rm c}(k;q)$ is an even function of q for the type-b boundary field. Indeed, we have

$$\delta_{\rm c}^{-}(k;q) = \begin{cases} \dfrac{1}{\rm i}\ln\dfrac{1-q{\rm e}^{{\rm i}k}}{1-q{\rm e}^{-{\rm i}k}} + \Theta_{\rm c}(k;q) & \text{for type } a \\ \dfrac{1}{\rm i}\ln\left(\dfrac{1+q{\rm e}^{{\rm i}k}}{1+q{\rm e}^{-{\rm i}k}}\dfrac{\Gamma\left(\frac{1}{2}\xi+\frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)-\frac{1}{2}{\rm i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi-\frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)+\frac{1}{2}{\rm i}\theta\right)}\right) & \\ \qquad\qquad + \Theta_{\rm c}(k;q) & \text{for type } b \end{cases} \tag{2.32}$$

for $1 > q > 0$ and $\xi > \frac{1}{2}$.

Then, we find that the following relationships hold:

$$\delta_{\rm c}^{-}(k;q) - \delta_{\rm c}^{+}(k;q) = \begin{cases} \dfrac{1}{\rm i}\ln\dfrac{\xi-{\rm i}\theta}{\xi+{\rm i}\theta} & \text{for type } a \\ 0 & \text{type } b. \end{cases} \tag{2.33}$$

2.4. Spin sector

In this subsection, we determine the scattering matrices for the elementary excitation of the spin sector for $u > 0$.

In this case, we consider the quantization condition for factorized scattering of two-particle states with rapidities λ_1 and λ_2;

$$\exp\left({\rm i}p_{\rm s}(\lambda_1)2\overline{L}\right) S_{\rm ss}(\theta_1-\theta_2)K_{\rm s}(\lambda_1;q_1)S_{\rm ss}(\theta_1+\theta_2)K_{\rm s}(\lambda_1;q_L) = 1 \tag{2.34}$$

with $\theta_j \equiv \lambda_j/(2u)$ for $j = 1, 2$. Here the symbol $p_{\rm s}(\lambda)$ denotes the momentum of a spinon of a rapidity λ. For the triplet state ($S = 1$), the bulk scattering matrix $S_{\rm ss}$ takes the form [1]

$$S_{\rm ss}(\mu) = {\rm e}^{{\rm i}\psi_{\rm ss}(\mu)} \qquad \psi_{\rm ss}(\mu) = \pi + \frac{1}{\rm i}\ln\left(\frac{\Gamma\left(\frac{1}{2}+\frac{1}{2}{\rm i}\mu\right)\Gamma\left(1-\frac{1}{2}{\rm i}\mu\right)}{\Gamma\left(\frac{1}{2}-\frac{1}{2}{\rm i}\mu\right)\Gamma\left(1+\frac{1}{2}{\rm i}\mu\right)}\right). \tag{2.35}$$

When we parametrize the boundary scattering matrix $K_{\rm s}(\lambda;q)$ as follows:

$$K_{\rm s}(\lambda;q) = \begin{pmatrix} \exp\left({\rm i}\phi_{\rm s}^{+}(\lambda;q)\right) & 0 \\ 0 & \exp\left({\rm i}\phi_{\rm s}^{-}(\lambda;q)\right) \end{pmatrix} \tag{2.36}$$

we can rewrite the quantization condition as

$$2\overline{L}p_{\rm s}(\lambda_1) + \psi_{\rm ss}(\theta_1-\theta_2) + \phi_{\rm s}^{\pm}(\lambda_1;q_1) + \psi_{\rm ss}(\theta_1+\theta_2) + \phi_{\rm s}^{\pm}(\lambda_1;q_L) = 0 \pmod{2\pi} \tag{2.37}$$

for two-particle states with $S^z = \pm 1$, respectively.

Within the string hypothesis, the state with $S^z = 1$ corresponds to that with two holes in the sea of real roots of $\{\lambda_\alpha\}$ and without holes in the sea of real $\{k_j\}$, i.e. $N = L$, $M_1 = L/2 - 1$, $M_n = 0$ ($n \geqslant 2$)) and $M_n' = 0$ ($n \geqslant 1$) . Then, the Bethe-ansatz equations are of the form

$$\frac{I_j}{L} = z_{\rm c}(k_j) \qquad \text{and} \qquad \frac{J_\alpha}{L} = z_{\rm s}(\lambda_\alpha) \tag{2.38}$$

$$2\pi z_{\rm c}(k) \equiv 2\left(1+\frac{1}{L}\right)k - \frac{\rm i}{L}\ln Z(k) + \frac{1}{L}\sum_{\beta=1}^{L/2+1}\left\{\theta\left(\frac{\sin k-\lambda_\beta}{u}\right)+\theta\left(\frac{\sin k+\lambda_\beta}{u}\right)\right\}$$
$$-\frac{1}{L}\sum_{\alpha=1}^{2}\left\{\theta\left(\frac{\sin k-\lambda_\alpha^{\rm h}}{u}\right)+\theta\left(\frac{\sin k+\lambda_\alpha^{\rm h}}{u}\right)\right\} \tag{2.39}$$

$$2\pi z_{\rm s}(\lambda) \equiv \frac{1}{L}\theta\left(\frac{\lambda}{u}\right) - \frac{\rm i}{L}\ln Y(\lambda) + \frac{1}{L}\sum_{l=1}^{L}\left\{\theta\left(\frac{\lambda-\sin k_l}{u}\right)+\theta\left(\frac{\lambda+\sin k_l}{u}\right)\right\}$$
$$-\frac{1}{L}\sum_{\beta=1}^{L/2+1}\left\{\theta\left(\frac{\lambda-\lambda_\beta}{2u}\right)+\theta\left(\frac{\lambda+\lambda_\beta}{2u}\right)\right\}$$
$$+\frac{1}{L}\sum_{\alpha=1}^{2}\left\{\theta\left(\frac{\lambda-\lambda_\alpha^{\rm h}}{2u}\right)+\theta\left(\frac{\lambda+\lambda_\alpha^{\rm h}}{2u}\right)\right\}. \tag{2.40}$$

Here $\{I_j\}$ $(j=1,\ldots,L)$ and $\{J_\alpha\}$ $(\alpha=1,\ldots,L/2+1)$ take positive integer values. Two of the $\{J_\alpha\}$ correspond to the holes with the rapidities $\lambda_1^{\rm h}$ and $\lambda_2^{\rm h}$. We neglect terms less than $1/L$ to obtain

$$2\pi z_{\rm s}(\lambda) = -2\left(1+\frac{1}{L}\right)(p_{\rm s}(\lambda)-p_{\rm s}(0)) - \frac{1}{L}(\mathcal{B}_{\rm s}(\lambda;q_1)+\mathcal{B}_{\rm s}(\lambda;q_L)) - \frac{1}{L}\Psi(\lambda)$$
$$+\frac{1}{L}\left\{\sum_{\alpha=1}^{2}\left(\Phi(\lambda-\lambda_\alpha^{\rm h})+\Phi(\lambda+\lambda_\alpha^{\rm h})\right)+\Phi(\lambda)\right\} \tag{2.41}$$

with

$$\mathcal{B}_{\rm s}(\lambda;q) = \frac{1}{\rm i}\int_{-\infty}^{\infty}\frac{{\rm d}\omega}{\omega}\frac{{\rm e}^{-{\rm i}\omega\lambda}{\rm e}^{u|\omega|}}{2\cosh u\omega}\tilde{\mathcal{A}}_{\rm R}(\omega;q). \tag{2.42}$$

Using the function $z_{\rm s}$ thus obtained, we can derive

$$-2\pi z_{\rm s}(\lambda_1)L = 2(L+1)(p_{\rm s}(\lambda_1)-p_{\rm s}(0)) - \Phi(\lambda_1-\lambda_2) - \Phi(\lambda_1+\lambda_2)$$
$$+\Psi(\lambda_1) - \Phi(\lambda_1) - \Phi(2\lambda_1) + \mathcal{B}_{\rm s}(\lambda_1;q_1) + \mathcal{B}_{\rm s}(\lambda_1;q_L) \tag{2.43}$$

where we use λ_α as an abbreviation for $\lambda_\alpha^{\rm h}$. Taking the equality

$$2\pi z_{\rm s}(\lambda_1)L = 0 \pmod{2\pi} \tag{2.44}$$

into account, equations (2.43) and (2.37) yield

$$\phi_{\rm s}^{+}(\lambda;q) = \phi_{\rm s}^{(0)}(\lambda) + \delta_{\rm s}^{+}(\lambda;q) \tag{2.45}$$

$$\phi_{\rm s}^{(0)}(\lambda) = \tfrac{1}{2}(\Psi(\lambda)-\Phi(\lambda)-\Phi(2\lambda)) \qquad \delta_{\rm s}^{+}(\lambda;q) = \mathcal{B}_{\rm s}(\lambda;q) \tag{2.46}$$

up to rapidity-independent additive constants. We have already derived $\phi_{\rm s}^{(0)}$ in [3]. The explicit forms of $\phi_{\rm s}^{(0)}$ and $\delta_{\rm s}^{+}$ are given by

$$\phi_{\rm s}^{(0)}(\lambda) = \frac{1}{\rm i}\ln\left(\frac{\Gamma\left(1-\frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{3}{4}+\frac{1}{2}{\rm i}\theta\right)}{\Gamma\left(1+\frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{3}{4}-\frac{1}{2}{\rm i}\theta\right)}\right) \qquad \theta = \frac{\lambda}{2u} \tag{2.47}$$

$$\delta_{\rm s}^{+}(\lambda;q) = \begin{cases} \Theta_{\rm s}(\lambda;q) & \text{for type } a \\ \frac{1}{\rm i}\ln\left(\frac{\Gamma\left(\frac{1}{2}\xi-\frac{1}{4}+\frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{1}{2}\xi+\frac{1}{4}-\frac{1}{2}{\rm i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi-\frac{1}{4}-\frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{1}{2}\xi+\frac{1}{4}+\frac{1}{2}{\rm i}\theta\right)}\right)+\Theta_{\rm s}(\lambda;q) & \text{for type } b \end{cases} \tag{2.48}$$

with $1 > q > 0$ and $\xi > \frac{1}{2}$, where

$$\Theta_{\rm s}(\lambda; q) = \frac{1}{\rm i}\int_{-\infty}^{\infty}\frac{{\rm d}\omega}{\omega}\,{\rm e}^{-{\rm i}\omega\lambda}\,\frac{1}{2\cosh u\omega}\left(2\sum_{j=1}^{\infty} q^{2j} J_{2j}(\omega)\right). \tag{2.49}$$

Next, in order to discuss the two-particle state with $S^z = -1$, we consider the canonical transformation

$$c_{j+} \longrightarrow c_{j-} \qquad \text{and} \qquad c_{j-} \longrightarrow c_{j+} \tag{2.50}$$

which keeps the Hamiltonian (1.1) without the boundary-field terms invariant. This transformation changes the sign of the type-b boundary field while it keeps the type-a boundary field invariant. The operators $\sum_{\alpha=x,y,z}\mathcal{T}^\alpha\mathcal{T}^\alpha$, $\mathcal{T}^z$ and $\sum_{\alpha=x,y,z}\mathcal{S}^\alpha\mathcal{S}^\alpha$ are invariant, and $\mathcal{S}^z$ changes into $-\mathcal{S}^z$. Hence, we can obtain the state with $S^z = -1$ of the Hubbard model (1.1) as that with $S^z = 1$ of the model with the type-b boundary field reversed. By taking this fact into account, we have

$$\phi_{\rm s}^-(\lambda; q) = \phi_{\rm s}^{(0)}(\lambda) + \delta_{\rm s}^-(\lambda; q) \qquad \delta_{\rm s}^+(\lambda; q) = \mathcal{B}_{\rm s}(\lambda; -q) \tag{2.51}$$

up to rapidity-independent additive constants. Here we remark that the function $\mathcal{B}_{\rm s}(\lambda; q)$ is even with respect to q for the type-a boundary field. The explicit form of the phase shift is given by

$$\delta_{\rm s}^-(\lambda; q) = \begin{cases} \Theta_{\rm s}(\lambda; q) & \text{for type } a \\ \dfrac{1}{\rm i}\ln\left(\dfrac{\Gamma\left(\frac{1}{2}\xi + \frac{3}{4} + \frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{1}{2}\xi + \frac{1}{4} - \frac{1}{2}{\rm i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi + \frac{3}{4} - \frac{1}{2}{\rm i}\theta\right)\Gamma\left(\frac{1}{2}\xi + \frac{1}{4} + \frac{1}{2}{\rm i}\theta\right)}\right) + \Theta_{\rm s}(\lambda; q) & \text{for type } b \end{cases} \tag{2.52}$$

for $1 > q > 0$ and $\xi > \frac{1}{2}$.

Finally, we arrive at the following relationships:

$$\delta_{\rm s}^-(\lambda; q) - \delta_{\rm s}^+(\lambda; q) = \begin{cases} 0 & \text{for type } a \\ \dfrac{1}{\rm i}\ln\dfrac{\xi - \frac{1}{2} + {\rm i}\theta}{\xi - \frac{1}{2} - {\rm i}\theta} & \text{for type } b. \end{cases} \tag{2.53}$$

3. Attractive Hubbard open chain

3.1. Review of the bulk scattering matrix

In this subsection, we briefly review the two-body scattering matrix in the bulk for the attractive Hubbard chain [1, 2]. (For detailed discussions, see, e.g., [1, 2] and references therein.)

The attractive Hubbard model has also four elementary excitations, which form a fundamental representation of $SU(2)_{\rm spin} \times SU(2)_{\rm charge}$ [1, 2]. Two of them are chargeless spin-carriers with the quantum numbers $S = \frac{1}{2}$, $S^z = \pm\frac{1}{2}$ and $T = 0$. The dispersion relations of these quasiparticles are given by

$$p_1(k) = k - \int_0^{\infty}\frac{{\rm d}\omega}{\omega}\,\frac{J_0(\omega)\sin(\omega\sin k)\,{\rm e}^{-\omega|u|}}{\cosh(\omega u)} \tag{3.1}$$

$$\varepsilon_1(k) = 2|u| - 2\cos k + 2\int_0^{\infty}\frac{{\rm d}\omega}{\omega}\,\frac{J_1(\omega)\cos(\omega\sin k)\,{\rm e}^{-\omega|u|}}{\cosh(\omega u)}. \tag{3.2}$$

The other two elementary excitations are spinless charge-carriers with the quantum numbers $T = \frac{1}{2}$, $T^z = \pm\frac{1}{2}$ and $S = 0$. These particles have the following dispersion relations:

$$p_2^{\mathrm{p}}(\lambda) = \pi - \int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_0(\omega)\sin(\omega\lambda)}{\cosh(\omega u)} = \pi + p_2^{\mathrm{h}}(\lambda) \tag{3.3}$$

$$\varepsilon_2^{\mathrm{p}}(\lambda) = 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega} \frac{J_1(\omega)\cos(\omega\lambda)}{\cosh(\omega u)} = \varepsilon_2^{\mathrm{h}}(\lambda). \tag{3.4}$$

Here the charge excitation with $T^z = \frac{1}{2}$ ($T^z = -\frac{1}{2}$) has the momentum $p_2^{\mathrm{h}}(\lambda)$ ($p_2^{\mathrm{p}}(\lambda)$) and the energy $\varepsilon_2^{\mathrm{h}}(\lambda)$ ($\varepsilon_2^{\mathrm{p}}(\lambda)$).

The two-body scattering matrix of these elementary excitations takes the following form:

$$S = \begin{pmatrix} S_{11}(\mu_1) & 0 & 0 & 0 \\ 0 & S_{12}(\mu_2) & 0 & 0 \\ 0 & 0 & S_{21}(\mu_3) & 0 \\ 0 & 0 & 0 & S_{22}(\mu_4) \end{pmatrix}. \tag{3.5}$$

At first, the matrix S_{11} describes the scattering of two spin-carriers (with rapidities k_1 and k_2), which is of the form

$$S_{11}(\mu) = \frac{\Gamma\left(\frac{1}{2} - \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 + \frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2} + \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 - \frac{1}{2}\mathrm{i}\mu\right)}\left(\frac{\mu\mathcal{I} - \mathrm{i}\mathcal{P}}{\mu - \mathrm{i}}\right) \qquad \mu = \frac{\sin k_1 - \sin k_2}{2|u|} \quad (> 0). \tag{3.6}$$

Next, the matrix S_{22} describing scattering of two charge-carriers (with rapidities λ_1 and λ_2) takes the following form:

$$S_{22}(\mu) = -\frac{\Gamma\left(\frac{1}{2} + \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 - \frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2} - \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 + \frac{1}{2}\mathrm{i}\mu\right)}\left(\frac{\mu\mathcal{I} + \mathrm{i}\mathcal{P}}{\mu + \mathrm{i}}\right) \qquad \mu = \frac{\lambda_1 - \lambda_2}{2|u|} \quad (> 0). \tag{3.7}$$

The scattering of one spin-carrier and one charge-carrier is described by

$$S_{12}(\mu) = -\mathrm{i}\frac{1 + \mathrm{i}\exp(\pi\mu)}{1 - \mathrm{i}\exp(\pi\mu)}\mathcal{I} \qquad \mu = \frac{\sin k - \lambda}{2|u|} \quad (> 0) \tag{3.8}$$

$$S_{21}(\mu) = -\mathrm{i}\frac{1 + \mathrm{i}\exp(\pi\mu)}{1 - \mathrm{i}\exp(\pi\mu)}\mathcal{I} \qquad \mu = \frac{\lambda - \sin k}{2|u|} \quad (> 0). \tag{3.9}$$

3.2. String hypothesis

In this subsection, we explain the string hypothesis [1, 14] for the attractive Hubbard chain. Within this hypothesis, we calculate the boundary scattering matrices in subsections 3.3 and 3.4.

For the attractive Hubbard chain, we assume that the solutions for the Bethe-ansatz equations take the following string forms [1, 14].

(1) λ-strings: n λ_α's combine into a string-type configuration to take the form

$$\lambda_\alpha^{n,j} = \lambda_\alpha^n + \mathrm{i}(n + 1 - 2j)|u| \qquad j = 1, \ldots, n \quad \alpha = 1, \ldots, M_n$$

with a real number λ_α^n, apart from a correction of order $\mathrm{e}^{-\delta L}$. Here δ is a positive number.
(2) k–λ-strings: $2n$ k_j's and n λ_α's combine into another string-type configuration and take the following forms within the accuracy of $\mathrm{O}(\mathrm{e}^{-\delta L})$:

$$\lambda'^{n,j}_\alpha = \lambda'^n_\alpha + \mathrm{i}(n + 1 - 2j)|u| \qquad j = 1, \ldots, n \quad \alpha = 1, \ldots, M'_n$$

with a real number λ'^{n}_{α}, and

$$k^1_\alpha = \sin^{-1}(\lambda'^{n}_{\alpha} + \mathrm{i}n|u|)$$

$$k^2_\alpha = \sin^{-1}(\lambda'^{n}_{\alpha} + \mathrm{i}(n-2)|u|) \qquad k^3_\alpha = \pi - k^2_\alpha$$

$$k^4_\alpha = \sin^{-1}(\lambda'^{n}_{\alpha} + \mathrm{i}(n-4)|u|) \qquad k^5_\alpha = \pi - k^4_\alpha$$

$$\vdots$$

$$k^{2n-2}_\alpha = \sin^{-1}(\lambda'^{n}_{\alpha} - \mathrm{i}(n-2)|u|) \qquad k^{2n-1}_\alpha = \pi - k^{2n-2}_\alpha$$

$$k^{2n}_\alpha = \sin^{-1}(\lambda'^{n}_{\alpha} - \mathrm{i}n|u|).$$

(3) Real k_j's, which do not form the above string-type configurations. (Hereafter, we describe only this type of real element in $\{k_j\}$ by the symbols k_j.)

If we introduce the number M' by $M' = \sum_{n=1}^{\infty} nM'_n$, the number of real k_j's is equal to $N - 2M'$. We also find that the relationship $M = \sum_{n=1}^{\infty} nM_n + \sum_{n=1}^{\infty} nM'_n$ holds.

The ground state of the present model (1.1) with $u < 0$ corresponds to the case with $N = L$, $M'_1 = L/2$, $M'_n = 0$ ($n \geqslant 2$) and $M_n = 0$ ($n \geqslant 1$).

3.3. Spin sector

In this subsection, we derive the boundary scattering matrices for the elementary excitation with spin for the attractive Hubbard chain.

The quantization condition for factorized scattering of such two particles with rapidities k_1 and k_2 on a line of length $\bar{L}$ is given by

$$\exp\left(\mathrm{i}p_1(k_1)2\bar{L}\right) S_{11}(\theta_1 - \theta_2) K_1(k_1; q_1) S_{11}(\theta_1 + \theta_2) K_1(k_1; q_L) = 1 \qquad (3.10)$$

with $\theta_j \equiv \sin k_j/(2|u|)$ for $j = 1, 2$. For the triplet state ($S = 1$), the bulk scattering matrix S_{11} take the form [1]

$$S_{11}(\mu) = \mathrm{e}^{\mathrm{i}\psi_{11}(\mu)} \qquad \psi_{11}(\mu) = \frac{1}{\mathrm{i}} \ln\left(\frac{\Gamma\left(\frac{1}{2} - \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 + \frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2} + \frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1 - \frac{1}{2}\mathrm{i}\mu\right)}\right). \qquad (3.11)$$

We can rewrite the quantization conditions as

$$2\bar{L}p_1(k) + \psi_{11}(\theta_1 - \theta_2) + \phi_1^{\pm}(k_1; q_1) + \psi_{11}(\theta_1 + \theta_2) + \phi_1^{\pm}(k_1; q_L) = 0 \pmod{2\pi} \quad (3.12)$$

for the states with $S^z = \pm 1$, where we have parametrized the boundary scattering matrices K_1 as follows:

$$K_1(k; q) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\phi_1^+(k;q)} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\phi_1^-(k;q)} \end{pmatrix}. \qquad (3.13)$$

The two-particle state with $S^z = 1$ corresponds to the case with $N = L$, $M'_1 = L/2 - 1$, $M'_n = 0$ ($n \geqslant 2$) and $M_n = 0$ ($n \geqslant 1$). In this case, the Bethe-ansatz equations take the forms

$$\frac{I_j}{L} = z_1(k^{\mathrm{p}}_j) \qquad \text{and} \qquad \frac{J_\alpha}{L} = z_2(\lambda_\alpha) \qquad (3.14)$$

$$2\pi z_1(k) \equiv 2\left(1 + \frac{1}{L}\right)k - \frac{\mathrm{i}}{L}\ln Z(k) - \frac{1}{L}\sum_{\beta=1}^{L/2-1}\left\{\theta\left(\frac{\sin k - \lambda_\beta}{|u|}\right) + \theta\left(\frac{\sin k + \lambda_\beta}{|u|}\right)\right\}$$

(3.15)

$$2\pi z_2(\lambda) \equiv 2\left(1+\frac{1}{L}\right)\left(\sin^{-1}(\lambda+\mathrm{i}|u|)+\sin^{-1}(\lambda-\mathrm{i}|u|)\right)-\frac{1}{L}\theta\left(\frac{\lambda}{|u|}\right)-\frac{\mathrm{i}}{L}\ln\overline{Y}(\lambda)$$
$$-\frac{1}{L}\sum_{j=1}^{2}\left\{\theta\left(\frac{\lambda-\sin k_j^{\mathrm{p}}}{|u|}\right)+\theta\left(\frac{\lambda+\sin k_j^{\mathrm{p}}}{|u|}\right)\right\}$$
$$-\frac{1}{L}\sum_{\beta=1}^{L/2-1}\left\{\theta\left(\frac{\lambda-\lambda_\beta}{2|u|}\right)+\theta\left(\frac{\lambda+\lambda_\beta}{2|u|}\right)\right\} \tag{3.16}$$

with

$$\overline{Y}(\lambda;q_1,q_2)\equiv Y(\lambda;q_1,q_2)Z(k^+;q_1,q_2)Z(k^-;q_1,q_2) \qquad \sin k^\pm \equiv \lambda\pm\mathrm{i}|u|. \tag{3.17}$$

Here $\{I_j\}$ $(j=1,2)$ and $\{J_\alpha\}$ $(\alpha=1,\ldots,L/2-1)$ take integer values. We have no holes in the sea of the real rapidities $\{\lambda_\alpha\}$ while the integers I_1 and I_2 correspond to the two particles with the real rapidities k_1^{p} and k_2^{p}. If we neglect higher-order terms of $1/L$, we can derive the explicit form of z_1 as follows:

$$2\pi z_1(k)=2\left(1+\frac{1}{L}\right)(p_1(k)-p_1(0))+\frac{1}{L}\left(\mathcal{B}_1(k;q_1)+\mathcal{B}_1(k;q_L)\right)+\frac{1}{L}\Psi(\sin k)$$
$$+\frac{1}{L}\left\{\sum_{j=1}^{2}\left(\Phi(\sin k-\sin k_j^{\mathrm{p}})+\Phi(\sin k+\sin k_j^{\mathrm{p}})\right)+\Phi(\sin k)\right\} \tag{3.18}$$

with

$$\mathcal{B}_1(k;q)=\frac{1}{\mathrm{i}}\ln\frac{1+q\mathrm{e}^{-\mathrm{i}k}}{1+q\mathrm{e}^{\mathrm{i}k}}+\frac{1}{\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\mathrm{e}^{-\mathrm{i}\omega\sin k}}{2\cosh u\omega}\tilde{\mathcal{A}}_{\mathrm{A}}(\omega;q). \tag{3.19}$$

Here $\tilde{\mathcal{A}}_{\mathrm{A}}(\omega;q)$ denotes the Fourier-transformed function of $\mathcal{A}_{\mathrm{A}}(\lambda;q)$, which is defined by

$$\mathcal{A}_{\mathrm{A}}(\lambda;q)=\begin{cases}\mathcal{A}_2(\lambda;q) & \text{for type } a\\ \mathcal{A}_1(\lambda;q)+\mathcal{A}_2(\lambda;q) & \text{for type } b\end{cases} \tag{3.20}$$

$$\mathcal{A}_2(\lambda;q)=\frac{1}{2\pi\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\left(\zeta(k^+;q)\zeta(k^-;q)\right). \tag{3.21}$$

The symbol $\mathcal{A}_{\mathrm{A}}(\lambda;q)$ is an abbreviation for $\mathcal{A}_{\mathrm{A}}^x(\lambda;q|u)$ with $x=a,b$. Here we can prove that the equations

$$\mathcal{A}_{\mathrm{A}}^a(\lambda;q|u)=\mathcal{A}_{\mathrm{R}}^b(\lambda;-q|\ |u|\ ) \qquad \text{and} \qquad \mathcal{A}_{\mathrm{A}}^b(\lambda;q|u)=\mathcal{A}_{\mathrm{R}}^a(\lambda;-q|\ |u|\ ) \tag{3.22}$$

hold for $|q|<1$. In the following calculation, we take these relationships into account. (We have already derived and used these equalities in [15].)

We compare the quantization condition (3.12) with the relationship

$$2\pi z_1(k_1)L=0 \quad (\mathrm{mod}\ 2\pi) \tag{3.23}$$

$$2\pi z_1(k_1)L=2(L+1)(p_1(k)-p_1(0))+\Phi(\sin k_1-\sin k_2)+\Phi(\sin k_1+\sin k_2)$$
$$+\Psi(\sin k)+\Phi(\sin k)+\Phi(2\sin k)+\mathcal{B}_1(k_1;q_1)+\mathcal{B}_1(k_1;q_L) \tag{3.24}$$

(where we describe $\{k_j^{\mathrm{p}}\}$ by the symbols k_j as abbreviations), so that we obtain

$$\phi_1^+(k;q)=\phi_1^{(0)}(k)+\delta_1^+(k;q) \tag{3.25}$$

$$\phi_1^{(0)}(k)=\tfrac{1}{2}\left(\Psi(\sin k)+\Phi(\sin k)+\Phi(2\sin k)\right) \qquad \delta_1^+(k;q)=\mathcal{B}_1(k;q) \tag{3.26}$$

apart from rapidity-independent constants. We can find explicit forms of the phase shifts as follows:

$$\phi_1^{(0)}(k) = \frac{1}{\mathrm{i}} \ln \left(\frac{\Gamma\left(1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{4}-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{4}+\frac{1}{2}\mathrm{i}\theta\right)} \right) \qquad \theta = \frac{\sin k}{2|u|} \tag{3.27}$$

$$\delta_1^+(k;q) = \begin{cases} \frac{1}{\mathrm{i}} \ln \left(\frac{1+q\mathrm{e}^{-\mathrm{i}k}}{1+q\mathrm{e}^{\mathrm{i}k}} \frac{\Gamma\left(\frac{1}{2}\xi+1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi+1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)+\frac{1}{2}\mathrm{i}\theta\right)} \right) & \\ \qquad + \Theta_1(k;q) & \text{for type } a \\ \frac{1}{\mathrm{i}} \ln \frac{1+q\mathrm{e}^{-\mathrm{i}k}}{1+q\mathrm{e}^{\mathrm{i}k}} + \Theta_1(k;q) & \text{for type } b \end{cases} \tag{3.28}$$

for $1 > q > 0$ and $2\xi \equiv (q^{-1} - q)/(2|u|) > 1$. Here we have defined the function Θ_1 as follows:

$$\Theta_1(k;q) = \frac{1}{\mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\omega} \mathrm{e}^{-\mathrm{i}\omega \sin k} \frac{\mathrm{e}^{-|u\omega|}}{2\cosh u\omega} \left(2 \sum_{j=1}^{\infty} q^{2j} J_{2j}(\omega) \right). \tag{3.29}$$

By an argument similar to that in subsection 2.4, we obtain the case with $S^z = -1$ to derive the boundary phase shifts

$$\phi_1^-(k;q) = \phi_1^{(0)}(k) + \delta_1^-(k;q) \qquad \delta_1^-(k;q) = \mathcal{B}_1(k;-q) \tag{3.30}$$

with

$$\delta_1^-(k;q) = \begin{cases} \frac{1}{\mathrm{i}} \ln \left(\frac{1+q\mathrm{e}^{-\mathrm{i}k}}{1+q\mathrm{e}^{\mathrm{i}k}} \frac{\Gamma\left(\frac{1}{2}\xi+1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi+1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}(\xi+1)+\frac{1}{2}\mathrm{i}\theta\right)} \right) & \\ \qquad + \Theta_1(k;q) & \text{for type } a \\ \frac{1}{\mathrm{i}} \ln \frac{1-q\mathrm{e}^{-\mathrm{i}k}}{1-q\mathrm{e}^{\mathrm{i}k}} + \Theta_1(k;q) & \text{for type } b \end{cases} \tag{3.31}$$

for $1 > q > 0$ and $2\xi > 1$.

The difference between the phase shifts for the quasiparticles with $S^z = \frac{1}{2}$ and $S^z = -\frac{1}{2}$ is given by

$$\delta_1^-(k;q) - \delta_1^+(k;q) = \begin{cases} 0 & \text{for type } a \\ \frac{1}{\mathrm{i}} \ln \frac{\xi + \mathrm{i}\theta}{\xi - \mathrm{i}\theta} & \text{for type } b. \end{cases} \tag{3.32}$$

3.4. Charge sector

In this subsection, we derive the boundary scattering matrices for the elementary excitations with charge for the attractive Hubbard chain.

The quantization condition for factorized scattering of two-particle states with rapidities λ_1 and λ_2 are given by

$$\exp\left(\mathrm{i}p_2(\lambda_1)2\overline{L}\right) S_{22}(\theta_1 - \theta_2) K_2(\lambda_1; q_1) S_{22}(\theta_1 + \theta_2) K_2(\lambda_1; q_L) = 1 \tag{3.33}$$

with $\theta_j \equiv \lambda_j/(2|u|)$ for $j=1,2$. We take $p_2^{\mathrm{h}}(\lambda)$ ($p_2^{\mathrm{p}}(\lambda)$) as $p_2(\lambda)$ for the particle with $T^z=\frac{1}{2}$ ($T^z=-\frac{1}{2}$). For the two-particle state with $T=1$, the bulk scattering matrix is of the form

$$S_{22}(\mu)=\mathrm{e}^{\mathrm{i}\psi_{22}(\mu)} \qquad \psi_{22}=\pi+\frac{1}{\mathrm{i}}\ln\left(\frac{\Gamma\left(\frac{1}{2}+\frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1-\frac{1}{2}\mathrm{i}\mu\right)}{\Gamma\left(\frac{1}{2}-\frac{1}{2}\mathrm{i}\mu\right)\Gamma\left(1+\frac{1}{2}\mathrm{i}\mu\right)}\right). \tag{3.34}$$

Then the quantization condition take the following forms:

$$2\overline{L}p_2^{\mathrm{h}}(\lambda_1)+\psi_{22}(\theta_1-\theta_2)+\phi_2^{+}(\lambda_1;q_1)+\psi_{22}(\theta_1+\theta_2)+\phi_2^{+}(\lambda_1;q_L)=0 \pmod{2\pi} \tag{3.35}$$

for $T^z=1$, and

$$2\overline{L}p_2^{\mathrm{p}}(\lambda_1)+\psi_{22}(\theta_1-\theta_2)+\phi_2^{-}(\lambda_1;q_1)+\psi_{22}(\theta_1+\theta_2)+\phi_2^{-}(\lambda_1;q_L)=0 \pmod{2\pi} \tag{3.36}$$

for $T^z=-1$, where $\phi_2^{\pm}$ are introduced as follows:

$$K_2(\lambda;q)=\begin{pmatrix}\mathrm{e}^{\mathrm{i}\phi_2^{+}(\lambda;q)} & 0\\ 0 & \mathrm{e}^{\mathrm{i}\phi_2^{-}(\lambda;q)}\end{pmatrix}. \tag{3.37}$$

In order to determine ϕ_2^{+}, we consider the two-particle state with $T^z=1$. This state corresponds to the case with $N=L-2$, $M_1'=L/2-1$, $M_n'=0$ ($n\geqslant 2$) and $M_n=0$ ($n\geqslant 1$). In this case, we have no real rapidities described by k_j to rewrite the Bethe-ansatz equations in the following form:

$$\frac{J_\alpha}{L}=z_2(\lambda_\alpha) \tag{3.38}$$

$$\begin{aligned}2\pi z_2(\lambda)\equiv{}&2\left(1+\frac{1}{L}\right)\left(\sin^{-1}(\lambda+\mathrm{i}|u|)+\sin^{-1}(\lambda-\mathrm{i}|u|)\right)-\theta\left(\frac{\lambda}{|u|}\right)-\frac{\mathrm{i}}{L}\ln\overline{Y}(\lambda)\\ &-\frac{1}{L}\sum_{\beta=1}^{L/2+1}\left\{\theta\left(\frac{\lambda-\lambda_\beta}{2|u|}\right)+\theta\left(\frac{\lambda+\lambda_\beta}{2|u|}\right)\right\}\\ &+\frac{1}{L}\sum_{\alpha=1}^{2}\left\{\theta\left(\frac{\lambda-\lambda_\alpha^{\mathrm{h}}}{2|u|}\right)+\theta\left(\frac{\lambda+\lambda_\alpha^{\mathrm{h}}}{2|u|}\right)\right\}.\end{aligned} \tag{3.39}$$

Here $\{J_\alpha\}$ ($\alpha=1,\ldots,L/2+1$) take positive integer values, two of which correspond to the holes with the rapidities λ_1^{h} and λ_2^{h}. Then we obtain an explicit form of the function z_2 as follows:

$$\begin{aligned}2\pi z_2(\lambda)={}&-2\left(1+\frac{1}{L}\right)(p_2(\lambda)-p_2(0))-\frac{1}{L}\left(\mathcal{B}_2(\lambda;q_1)+\mathcal{B}_2(\lambda;q_L)\right)-\frac{1}{L}\Psi(\lambda)\\ &+\frac{1}{L}\left\{\sum_{\alpha=1}^{2}\left(\Phi(\lambda-\lambda_\alpha^{\mathrm{h}})+\Phi(\lambda+\lambda_\alpha^{\mathrm{h}})\right)+\Phi(\lambda)\right\}\end{aligned} \tag{3.40}$$

(where we have neglected higher order terms in $1/L$) with

$$\mathcal{B}_2(\lambda)=\frac{1}{\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\mathrm{e}^{-\mathrm{i}\omega\lambda}\mathrm{e}^{|u\omega|}}{2\cosh u\omega}\tilde{\mathcal{A}}_{\mathrm{A}}(\omega;q). \tag{3.41}$$

Then, we have the following equalities:

$$2\pi z_2(\lambda_2)L = 0 \pmod{2\pi} \tag{3.42}$$

$$\begin{aligned} -2\pi L z_2(\lambda_1) &= 2(L+1)\left(p_2(\lambda_1) - p_2(0)\right) - \Phi(\lambda_1 - \lambda_2) - \Phi(\lambda_1 + \lambda_2) \\ &\quad + \Psi(\lambda_1) - \Phi(\lambda_1) - \Phi(2\lambda_1) + \mathcal{B}_2(\lambda_1; q_1) + \mathcal{B}_2(\lambda_1; q_L) \end{aligned} \tag{3.43}$$

where we have used λ_α as an abbreviation for $\lambda_\alpha^{\mathrm{h}}$. Using the quantization condition (3.34), we can read off the phase shifts from equations (3.41), (3.42) as follows:

$$\phi_2^+(\lambda; q) = \phi_2^{(0)}(\lambda) + \delta_2^+(\lambda; q) \tag{3.44}$$

$$\phi_2^{(0)}(\lambda) = \tfrac{1}{2}\left(\Psi(\lambda) - \Phi(\lambda) - \Phi(2\lambda)\right) \qquad \delta_2^+(\lambda; q) = \mathcal{B}_2(\lambda; q) \tag{3.45}$$

up to rapidity-independent additive constants. The explicit forms of the phase shifts are given by

$$\phi_2^{(0)}(\lambda) = \frac{1}{\mathrm{i}} \ln\left(\frac{\Gamma\left(1 - \frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{3}{4} + \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1 + \frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{3}{4} - \frac{1}{2}\mathrm{i}\theta\right)}\right) \qquad \theta = \frac{\lambda}{2|u|} \tag{3.46}$$

$$\delta_2^+(\lambda; q) = \begin{cases} \dfrac{1}{\mathrm{i}} \ln\left(\dfrac{\Gamma\left(\frac{1}{2}\xi + \frac{3}{4} + \frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi + \frac{1}{4} - \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi + \frac{3}{4} - \frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi + \frac{1}{4} + \frac{1}{2}\mathrm{i}\theta\right)}\right) + \Theta_2(\lambda; q) & \text{for type } a \\ \Theta_2(\lambda; q) & \text{for type } b \end{cases} \tag{3.47}$$

for $1 > q > 0$ and $2\xi > 1$, where

$$\Theta_2(\lambda; q) = \frac{1}{\mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\omega} \mathrm{e}^{-\mathrm{i}\omega\lambda} \frac{1}{2\cosh u\omega} \left(2 \sum_{j=1}^{\infty} q^{2j} J_{2j}(\omega)\right). \tag{3.48}$$

By an argument similarly to that in subsection 2.3, we can construct the two-particle state with $T^z = -1$. Then, we can also derive the phase shift $\phi_2^-(\lambda; q)$ as follows:

$$\phi_2^-(\lambda; q) = \phi_2^{(0)}(\lambda) + \delta_2^-(\lambda; q) \qquad \delta_2^-(\lambda; q) = \mathcal{B}_2(\lambda; -q) \tag{3.49}$$

or, more explicitly,

$$\delta_2^-(\lambda; q) = \begin{cases} \Theta_2(\lambda; q) & \text{for type } a \\ \dfrac{1}{\mathrm{i}} \ln\left(\dfrac{\Gamma\left(\frac{1}{2}\xi - \frac{1}{4} + \frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi + \frac{1}{4} - \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi - \frac{1}{4} - \frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi + \frac{1}{4} + \frac{1}{2}\mathrm{i}\theta\right)}\right) + \Theta_2(\lambda; q) & \text{for type } b \end{cases} \tag{3.50}$$

for $1 > q > 0$ and $2\xi > 1$.

Finally, we can arrive at the following relationships:

$$\delta_2^-(\lambda; q) - \delta_2^+(\lambda; q) = \begin{cases} 0 & \text{for type } a \\ \dfrac{1}{\mathrm{i}} \ln \dfrac{\xi - \frac{1}{2} - \mathrm{i}\theta}{\xi + \frac{1}{2} + \mathrm{i}\theta} & \text{for type } b. \end{cases} \tag{3.51}$$

4. Summary

In the present paper, we have determined the boundary scattering matrices of the Hubbard open chain with boundary fields. For each of the type-a and type-b boundary fields, the boundary scattering is described by 4×4 matrices. We summarize the results obtained by our calculations as follows.

4.1. Repulsive Hubbard open chain

In the repulsive Hubbard model, the boundary scattering matrix obtained by our calculations takes the form

$$K = \begin{pmatrix} K_{\mathrm{s}} & 0 \\ 0 & K_{\mathrm{c}} \end{pmatrix} \tag{4.1}$$

where the 2×2 matrix K_{s} (K_{c}) is diagonal and corresponds to the quasiparticle with spin (charge). The matrix K_{s} (K_{c}) is represented in the two-dimensional space spanned by the states with $S^z = \pm\frac{1}{2}$ ($T^z = \pm\frac{1}{2}$).

Type-a boundary boundary field.

$$K_{\mathrm{s}} = K_{\mathrm{s}}^{(0)}(\theta) K_{\mathrm{s}}^{(1)}(\theta; q) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \theta \equiv \frac{\lambda}{2u} \tag{4.2}$$

$$K_{\mathrm{c}} = K_{\mathrm{c}}^{(0)}(\theta) K_{\mathrm{c}}^{(1)}(\theta; q) \frac{1 + q\mathrm{e}^{\mathrm{i}k}}{1 + q\mathrm{e}^{-\mathrm{i}k}} \begin{pmatrix} 1 & 0 \\ 0 & \dfrac{\xi - \mathrm{i}\theta}{\xi + \mathrm{i}\theta} \end{pmatrix} \qquad \theta \equiv \frac{\sin k}{2u}. \tag{4.3}$$

Type-b boundary boundary field.

$$K_{\mathrm{s}} = K_{\mathrm{s}}^{(0)}(\theta) K_{\mathrm{s}}^{(1)}(\theta; q) \frac{\Gamma\left(\frac{1}{2}\xi - \frac{1}{4} + \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{1}{2}\xi + \frac{1}{4} - \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi - \frac{1}{4} - \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{1}{2}\xi + \frac{1}{4} + \frac{1}{2}\mathrm{i}\theta\right)} \begin{pmatrix} 1 & 0 \\ 0 & \dfrac{\xi - \frac{1}{2} + \mathrm{i}\theta}{\xi - \frac{1}{2} - \mathrm{i}\theta} \end{pmatrix}$$
$$\theta \equiv \frac{\lambda}{2u} \tag{4.4}$$

$$K_{\mathrm{c}} = K_{\mathrm{c}}^{(0)}(\theta) K_{\mathrm{c}}^{(1)}(\theta; q) \frac{1 + q\mathrm{e}^{\mathrm{i}k}}{1 + q\mathrm{e}^{-\mathrm{i}k}} \frac{\Gamma\left(\frac{1}{2}\xi + \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{1}{2}\xi + \frac{1}{2} - \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi - \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{1}{2}\xi + \frac{1}{2} + \frac{1}{2}\mathrm{i}\theta\right)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$\theta \equiv \frac{\sin k}{2u} \tag{4.5}$$

for $1 > q > 0$ and $2\xi \equiv (q^{-1} - q)/(2u)$ (> 1). Here we have defined the functions $K_{\mathrm{s}}^{(0)}$, $K_{\mathrm{s}}^{(1)}$, $K_{\mathrm{c}}^{(0)}$, $K_{\mathrm{c}}^{(1)}$ as follows:

$$K_{\mathrm{s}}^{(0)}(\theta) = \frac{\Gamma\left(1 - \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{3}{4} + \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1 + \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{3}{4} - \frac{1}{2}\mathrm{i}\theta\right)} \tag{4.6}$$

$$K_{\mathrm{c}}^{(0)}(\theta) = \frac{\Gamma\left(1 + \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{1}{4} - \frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1 - \frac{1}{2}\mathrm{i}\theta\right) \Gamma\left(\frac{1}{4} + \frac{1}{2}\mathrm{i}\theta\right)} \tag{4.7}$$

$$K_{\mathrm{s}}^{(1)}(\theta) = \exp\left[-\mathrm{i} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{\omega} \frac{\sin \omega\theta}{2\cosh \frac{\omega}{2}} \left(2 \sum_{j=1}^{\infty} q^{2j} J_{2j}\left(\frac{\omega}{2u}\right)\right)\right] \tag{4.8}$$

and

$$K_c^{(1)}(\theta) = \exp\left[-\mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\mathrm{e}^{-\frac{|\omega|}{2}}\sin\omega\theta}{2\cosh\frac{\omega}{2}}\left(2\sum_{j=1}^{\infty}q^{2j}J_{2j}\left(\frac{\omega}{2u}\right)\right)\right]. \tag{4.9}$$

4.2. Attractive Hubbard open chain

In the attractive Hubbard model, the boundary scattering matrix takes the following form:

$$K = \begin{pmatrix} K_1 & 0 \\ 0 & K_2 \end{pmatrix} \tag{4.10}$$

where the 2×2 matrix K_1 (K_2) is diagonal and corresponds to the quasiparticle with spin (charge).

Type-a boundary boundary field.

$$K_1 = K_1^{(0)}(\theta)K_1^{(1)}(\theta;q)\frac{1+q\mathrm{e}^{-\mathrm{i}k}}{1+q\mathrm{e}^{\mathrm{i}k}}\frac{\Gamma\left(\frac{1}{2}\xi+1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi+\frac{1}{2}-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi+1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi+\frac{1}{2}+\frac{1}{2}\mathrm{i}\theta\right)}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$\theta \equiv \frac{\sin k}{2|u|} \tag{4.11}$$

$$K_2 = K_2^{(0)}(\theta)K_2^{(1)}(\theta;q)\frac{\Gamma\left(\frac{1}{2}\xi+\frac{3}{4}+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi+\frac{1}{4}-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(\frac{1}{2}\xi+\frac{3}{4}-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{2}\xi+\frac{1}{4}+\frac{1}{2}\mathrm{i}\theta\right)}\begin{pmatrix} 1 & 0 \\ 0 & \dfrac{\xi-\frac{1}{2}-\mathrm{i}\theta}{\xi-\frac{1}{2}+\mathrm{i}\theta} \end{pmatrix}$$
$$\theta \equiv \frac{\lambda}{2|u|}. \tag{4.12}$$

Type-b boundary boundary field.

$$K_1 = K_1^{(0)}(\theta)K_1^{(1)}(\theta;q)\frac{1+q\mathrm{e}^{-\mathrm{i}k}}{1+q\mathrm{e}^{\mathrm{i}k}}\begin{pmatrix} 1 & 0 \\ 0 & \dfrac{\xi+\mathrm{i}\theta}{\xi-\mathrm{i}\theta} \end{pmatrix} \qquad \theta \equiv \frac{\sin k}{2|u|} \tag{4.13}$$

$$K_2 = K_2^{(0)}(\theta)K_2^{(1)}(\theta;q)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \theta \equiv \frac{\lambda}{2|u|} \tag{4.14}$$

for $1 > q > 0$ and $2\xi \equiv (q^{-1}-q)/(2|u|)$ (> 1). Here we have defined the functions $K_1^{(0)}$, $K_1^{(1)}$, $K_2^{(0)}$, $K_2^{(1)}$, as follows:

$$K_1^{(0)}(\theta) = \frac{\Gamma\left(1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{4}-\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{1}{4}+\frac{1}{2}\mathrm{i}\theta\right)} \tag{4.15}$$

$$K_2^{(0)}(\theta) = \frac{\Gamma\left(1-\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{3}{4}+\frac{1}{2}\mathrm{i}\theta\right)}{\Gamma\left(1+\frac{1}{2}\mathrm{i}\theta\right)\Gamma\left(\frac{3}{4}-\frac{1}{2}\mathrm{i}\theta\right)} \tag{4.16}$$

$$K_1^{(1)}(\theta) = \exp\left[-\mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\mathrm{e}^{-\frac{1}{2}|\omega|}\sin\omega\theta}{2\cosh\frac{1}{2}\omega}\left(2\sum_{j=1}^{\infty}q^{2j}J_{2j}\left(\frac{\omega}{2|u|}\right)\right)\right] \tag{4.17}$$

and

$$K_2^{(1)}(\theta) = \exp\left[-\mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\sin\omega\theta}{2\cosh\frac{1}{2}\omega}\left(2\sum_{j=1}^{\infty}q^{2j}J_{2j}\left(\frac{\omega}{2|u|}\right)\right)\right]. \tag{4.18}$$

We find that the type-a and the type-b boundary fields influence the boundary scattering matrices for both of the spin and the charge sectors. However, the matrices of the charge and the spin degrees of freedom are proportional to the identity matrices for the type-b and the type-a boundary fields, respectively. On the other hand, the a-type (b-type) boundary field sprits the charge doublet with $T = \frac{1}{2}$ (the spin doublet with $S = \frac{1}{2}$).

It is known [16] that in the scaling limit, the Hubbard chain with the $SO(4)$ symmetry is identified as the $SU(2)$ chiral-invariant Thirring (Gross–Neveu) model, containing massive and massless sectors (see, e.g., [17]). This scaling limit yields an integrable field theory with boundary interactions from the the Hubbard model with boundary fields. By taking an appropriate limit in the boundary scattering matrices of the Hubbard open chain, we may directly derive the matrices describing the boundary scattering [18] in the resulting field theory. Physical applications of the scattering matrices will be given in a separate paper.

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