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Elementary excitations in the Hubbard model with boundaries

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Abstract. Elementary excitations in the one-dimensional Hubbard model with boundaries are discussed at the half-filling and without external magnetic fields. The energy of the present model is evaluated in the low-lying excited state, where there exist quasiparticles corresponding to elementary excitations in the charge and the spin sectors. The boundary scattering matrix of the quasiparticles is evaluated.

1. Introduction

Recently, exactly solvable models with boundaries have attracted much attention. The one-dimensional Hubbard model with boundary fields is one of such strongly correlated systems. Schulz [1] has exactly diagonalized the Hubbard model with free boundaries by using the Bethe ansatz method. The present authors [2] derived the Bethe ansatz equation of the Hubbard open chain with a boundary field. Afterwards, several authors derived the Bethe ansatz equations with other boundary fields [3–5]. The physical properties of the Hubbard model with boundaries have been studied using the Bethe ansatz equations thus obtained. The finite-size scaling technique based on the boundary conformal field theory has enabled us to investigate critical behaviours of the present model with boundary fields [2–4] (see also [6]). The present authors have also evaluated the boundary contributions to physical quantities in the repulsive and the attractive Hubbard models with boundaries [7, 8]. In this paper, we discuss the elementary excitations in the Hubbard model on the open chain.

We study the present model at the half-filling without external magnetic fields in the bulk, which is described by the following Hamiltonian,

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

where $c_{j\sigma}^{\dagger}$ $(c_{j\sigma})$ denotes a fermionic creation (annihilation) operator at the site j with the spin σ, and $n_{j\sigma} = c_{j\sigma}^{\dagger}c_{j\sigma}$ denotes the number operator of the fermion. We take an even integer as L, which denotes the length of the open chain. The symbol $\mathcal{H}^{\mathrm{b}}$ corresponds to the boundary terms and takes the forms

$$\mathcal{H}^{\mathrm{b}} = \begin{cases} -p_1(n_{1+} + n_{1-} - 1) - p_L(n_{L+} + n_{L-} - 1) & \text{for case A} \\ -p_1(n_{1+} - n_{1-}) - p_L(n_{L+} - n_{L-}) & \text{for case B.} \end{cases} \tag{1.2}$$

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The energy of the present model is given by [2–5]

$$E = \sum_{j=1}^{N}(-2u - 2\cos k_j) + uL + e(p_1) + e(p_L) \tag{1.3}$$

with

$$e^{ik_j 2(L+1)} Z(k_j; p_1, p_L) = \prod_{\beta=1}^{M} \frac{\sin k_j - \lambda_\beta + iu}{\sin k_j - \lambda_\beta - iu} \frac{\sin k_j + \lambda_\beta + iu}{\sin k_j + \lambda_\beta - iu} \tag{1.4}$$

$$\prod_{l=1}^{N} \frac{\lambda_\alpha - \sin k_l + iu}{\lambda_\alpha - \sin k_l - iu} \frac{\lambda_\alpha + \sin k_l + iu}{\lambda_\alpha + \sin k_l - iu} = Y(\lambda_\alpha; p_1, p_L) \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{\lambda_\alpha - \lambda_\beta + i2u}{\lambda_\alpha - \lambda_\beta - i2u} \frac{\lambda_\alpha + \lambda_\beta + i2u}{\lambda_\alpha + \lambda_\beta - i2u} \tag{1.5}$$

for $j = 1, \ldots, N$ and $\alpha = 1, \ldots, M$, where N (or M) denotes the number of the fermions (or the fermions with down spins), and $e(p)$ takes p (or 0) for case A (or case B). Here, we define $Z(k_j; p_1, p_L)$ and $Y(\lambda_\alpha; p_1, p_L)$ by

$$Z(k; p_1, p_L) = \zeta(k; p_1)\zeta(k; p_L) \qquad \text{for cases A, B} \qquad \zeta(k; p) = \frac{1 - pe^{-ik_j}}{1 - pe^{ik_j}} \tag{1.6}$$

$$Y(\lambda; p_1, p_L) = \begin{cases} 1 & \text{for case A} \\ \eta(\lambda; p_1)\eta(\lambda; p_L) & \text{for case B} \end{cases} \qquad \eta(\lambda; p) = -\frac{\lambda + i(u + \frac{1}{2}(p^{-1} - p))}{\lambda - i(u + \frac{1}{2}(p^{-1} - p))}. \tag{1.7}$$

(In [2], the present authors have derived the Bethe ansatz equation for case A. One of the present authors (HA) [5] has derived the Bethe ansatz equation for case B from the equation for case A.)

We mainly discuss the case without the boundary fields ($p_1 = p_L = 0$), i.e. $\mathcal{H}^b = 0$. In this case, the Hamiltonian (1.1) (with $\mathcal{H}^b = 0$) is invariant under a $SO(4) = SU(2) \times SU(2)/Z_2$ transformation, similarly to the periodic-boundary case [9]. Namely, all the following six generators

$$S = \sum_{j=1}^{L} c_{j+}^\dagger c_{j-} \qquad S^\dagger = \sum_{j=1}^{L} c_{j-}^\dagger c_{j+} \qquad S^3 = \sum_{j=1}^{L} \tfrac{1}{2}(n_{j-} - n_{j+}) \tag{1.8}$$

$$T = \sum_{j=1}^{L} (-1)^j c_{j+} c_{j-} \qquad T^\dagger = \sum_{j=1}^{L} (-1)^j c_{j-}^\dagger c_{j+}^\dagger \qquad T^3 = \sum_{j=1}^{L} \tfrac{1}{2}(n_{j+} + n_{j-} - 1) \tag{1.9}$$

commute with the Hamiltonian $\mathcal{H}(u)$ with $\mathcal{H}^b = 0$. The Z_2 quotient corresponds to the fact that the operator $S^3 + T^3$ only has integer eigenvalues and all half-odd integer representations of the $SU(2) \times SU(2)$ are projected out, as L is even. Similarly to the periodic-boundary case, the partial particle–hole transformation

$$c_{j+} \longrightarrow (-1)^j c_{j+}^\dagger \qquad c_{j-} \longrightarrow c_{j-} \tag{1.10}$$

yields the change $\mathcal{H}(u) \to \mathcal{H}(-u)$ at the '$SO(4)$ point' (i.e. for $\mathcal{H}^b = 0$) and interchanges the charge and the spin degrees of freedom. Indeed, this transformation interchanges the spin-$SU(2)$ generators $\{S, S^\dagger, S^3\}$ and the charge-$SU(2)$ generators $\{T, T^\dagger, T^3\}$.

The elementary excitations in the Hubbard model with the *periodic* boundary condition have been discussed by many authors, e.g. [10–14], using the Bethe ansatz equation for the periodic Hubbard chain [10]. First, Lieb and Wu [10] showed that the repulsive Hubbard model at half-filling without magnetic field was an insulator for all positive values of u. Woynarovich [11] gave a detailed analysis of spin and charge excitations in the repulsive and the attractive Hubbard models. Klümper *et al* [12] rederived Woynarovich's result [11] using another method. Essler and Korepin [13] determined the two-particle scattering matrix for the elementary excitations. (Andrei [14] also discussed the scattering matrix.) These investigations have clarified the properties of the elementary excitations in the Hubbard model with the $SO(4)$ symmetry; (1) in the repulsive Hubbard model, charge and spin excitations are massive and massless, respectively. (2) In the attractive Hubbard model, spin and charge excitations are massive and massless, respectively. (3) In both the repulsive and the attractive cases, the excitation spectrum is built out of four elementary excitations (i.e. quasiparticles), which form the fundamental representation of $SU(2) \times SU(2)$. Two of these elementary excitations carry spin but no charge, and two carry charge but no spin.

In this paper, we have two aims. One of them is to derive the low-lying excited energy of the Hubbard open chain with the $SO(4)$ symmetry, where there exist several quasiparticles corresponding to elementary excitations in the charge and spin sectors. Woynarovich [11] has derived the low-lying excited energy with several quasiparticles for the periodic Hubbard chain (see also [12]). We extend his method [11] to derive the corresponding energy under the open boundary condition (sections 3.1, 3.2). As preliminaries for this calculation we have to discuss properties of the solutions in the Bethe ansatz equations (1.4) and (1.5) for the Hubbard model with boundaries (section 2).

The other aim is to derive the boundary scattering matrices for the quasiparticles of the Hubbard open chain with the $SO(4)$ symmetry (sections 4.1, 4.2).

Such boundary scattering matrices, which describe the phase shifts in the scattering of physical excitations at boundaries, have been evaluated in other models, e.g. [15–17]. Fendley and Saleur [15] and Grisaru *et al* [16] have derived the boundary scattering matrix for the Heisenberg open chain directly from the Bethe ansatz equation. Essler [17] has derived the scattering matrix for the supersymmetric t-J model, using Grisaru *et al*'s method [16]. Grisaru *et al*'s method [16] is based on the following quantization condition for factorized scattering of two particles with rapidities λ_1 and λ_2 on a line of length $\bar{L}$,

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

This condition comes from the requirement that the wavefunction should vanish at both ends of the line [15, 16]. Here, we describe the physical energy and the physical momentum of a 'dressed' particle (i.e. quasiparticle) with a rapidity λ by the symbols $\varepsilon(\lambda)$ and $p(\lambda)$. (We have to define $p(\lambda)$ by the physical momentum of the corresponding (infinite) periodic system [15, 16].) 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 off a boundary at the left (right) end. When the scattering matrices S_{12}, $K_1^{\mathrm{L(R)}}$ are proportional to the identity matrix, we can introduce phase shifts ψ_{12}, $\phi_1^{\mathrm{L(R)}}$ by

$$S_{12}(\lambda) = \mathrm{e}^{\mathrm{i}\psi_{12}(\lambda)} \qquad K_1^{\mathrm{L(R)}}(\lambda) = \mathrm{e}^{\mathrm{i}\phi_1^{\mathrm{L(R)}}(\lambda)} \tag{1.12}$$

(up to a rapidity-independent phase factor) to have the relationship

$$2\bar{L}p(\lambda_1) + \psi_{12}(\lambda_1-\lambda_2) + \phi_1^{\mathrm{L}}(\lambda_1) + \psi_{12}(\lambda_1+\lambda_2) + \phi_1^{\mathrm{R}}(\lambda_1) = 0 \qquad (\mathrm{mod}\ 2\pi) \tag{1.13}$$

apart from a rapidity-independent additive constant. For models on a one-dimensional lattice with L sites, we should take $L+1$ as $\bar{L}$. (For the free-fermion model, since each of the phase shifts ψ_{12}, $\phi_1^{\mathrm{L(R)}}$ is equal to zero, this relationship yields $p = \pi n/(L+1)$ ($n = 1, \ldots, L$). Indeed, the quantization condition for the free-fermion model on the open chain with L sites is given not by $p = \pi n/L$ but by $p = \pi n/(L+1)$.)

The quantization condition (1.11), i.e. (1.13), enables us to drive the boundary scattering matrix for the elementary excitations from the Bethe ansatz equation of the Hubbard model with boundaries. For detailed discussions, see sections 4.1 and 4.2.

2. Properties of the solutions for the Bethe ansatz equation of the Hubbard model with boundaries

In this section, we discuss properties of the solutions for the Bethe ansatz equations (1.4) and (1.5), as preliminaries for sections 3.1 and 3.2. The purpose of this section is to derive the 'complementary solutions' for the Bethe ansatz equations of the Hubbard model with boundaries. (Woynarovich [11] has derived the complementary solutions for the periodic-boundary case.)

If we require that solutions $\{k_j, \lambda_\alpha\}$ ($j = 1, \ldots, N$, $\alpha = 1, \ldots, M$) for the Bethe ansatz equations correspond to independent Bethe ansatz states, we can make the restrictions $-\frac{\pi}{2} < \arg k_j \leqslant \frac{\pi}{2}$ with $k_j \neq 0, \pi$, and $-\frac{\pi}{2} < \arg \lambda_\alpha \leqslant \frac{\pi}{2}$ with $\lambda_\alpha \neq 0$. We also have to identify $k_j + 2\pi$ as k_j (see [1, 2]).

Then, $-k_j$ and $-\lambda_\alpha$ also satisfy equations (1.4) and (1.5). If we define k_{-j} and $\lambda_{-\alpha}$ as $-k_j$ and $-\lambda_\alpha$ ($j = 1, \ldots, N$, $\alpha = 1, \ldots, M$), respectively, we have the relationships

$$\mathrm{e}^{\mathrm{i}k2(L+1)} Z(k_j; p_1, p_L) = \prod_{\beta=\pm1}^{\pm M} \frac{\sin k_j - \lambda_\beta + \mathrm{i}u}{\sin k_j - \lambda_\beta - \mathrm{i}u} \tag{2.1}$$

$$\prod_{l=\pm1}^{\pm N} \frac{\lambda_\alpha - \sin k_l + \mathrm{i}u}{\lambda_\alpha - \sin k_l - \mathrm{i}u} = Y(\lambda_\alpha; p_1, p_L) \left(-\frac{\lambda_\alpha + \mathrm{i}u}{\lambda_\alpha - \mathrm{i}u} \right)^{-1} \prod_{\beta=\pm1}^{\pm M} \frac{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u}$$
$$j = \pm1, \ldots, \pm N \qquad \alpha = \pm1, \ldots, \pm M. \tag{2.2}$$

For a fixed set $\{\lambda_\alpha\}$ ($\alpha = \pm1, \ldots, \pm M$), we can rewrite equation (2.1) as

$$P(x) = 0 \tag{2.3}$$

$$P(x) \equiv x^{2L}(x - p_1)(x - p_L) \prod_{\beta=\pm1}^{\pm M} (x^2 - 2\mathrm{i}(\lambda_\beta + \mathrm{i}u)x - 1)$$
$$-(1 - p_1 x)(1 - p_L x) \prod_{\beta=\pm1}^{\pm M} (x^2 - 2\mathrm{i}(\lambda_\beta - \mathrm{i}u)x - 1) \tag{2.4}$$

with $x = \mathrm{e}^{\mathrm{i}k_j}$. Then we can recognize $\{\mathrm{e}^{\mathrm{i}k_j}\}$ ($j = \pm1, \ldots, \pm N$) as $2N$ of $2L + 4M + 2$ roots for equation (2.3). We can check that $\mathrm{e}^{\mathrm{i}0}$ (i.e. 1) and $\mathrm{e}^{\mathrm{i}\pi}$ (i.e. -1) are also the roots of the equation. We can also check that the relation $P(x) = -x^{2L+4M+2} P(x^{-1})$ holds. Therefore, if x is a root of equation (2.3), x^{-1} is also a root of the equation. Now we parametrize the rest of the roots by $\{\mathrm{e}^{\mathrm{i}\tilde{k}_j}\}$ for $j = \pm1, \ldots, \pm N'$ ($N' \equiv L + 2M - N$) with $\tilde{k}_{-j} = -\tilde{k}_j$ for $j = 1, \ldots, N'$. (Here, we can recognize that the elements of $\{\mathrm{e}^{\mathrm{i}\tilde{k}_j}\}$ with $j = 1, \ldots, N'$ live on the half of the complex plane with $-\frac{\pi}{2} < \arg \tilde{k}_j \leqslant \frac{\pi}{2}$.) We call these roots $\{\tilde{k}_j\}$ ($j = \pm1, \ldots, \pm N'$) complementary solutions. By definition, the following relationships among $\{\tilde{k}_j\}$ ($j = \pm1 \ldots \pm N'$) and $\{\lambda_\alpha\}$ ($\alpha = \pm1 \ldots \pm M$) hold,

$$\mathrm{e}^{\mathrm{i}\tilde{k}2(L+1)} Z(\tilde{k}_j; p_1, p_L) = \prod_{\beta=\pm1}^{\pm M} \frac{\sin \tilde{k}_j - \lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j - \lambda_\beta - \mathrm{i}u}. \tag{2.5}$$

Introducing the parameters $x_j \equiv \mathrm{e}^{\mathrm{i}k_j}$ $(j = \pm 1, \ldots, \pm N)$ and $\tilde{x}_j \equiv \mathrm{e}^{\mathrm{i}\tilde{k}_j}$ $(j = \pm 1, \ldots, \pm N')$, we can rewrite equation (2.2) as

$$\sum_{l=\pm 1}^{\pm N} \frac{1}{\mathrm{i}} \ln \frac{x_l^2 - 2\mathrm{i}(\lambda_\alpha - \mathrm{i}u)x_l - 1}{x_l^2 - 2\mathrm{i}(\lambda_\alpha + \mathrm{i}u)x_l - 1} = -\frac{1}{\mathrm{i}} \ln Y(\lambda_\alpha; p_1, p_L) + \frac{1}{\mathrm{i}} \ln \left(-\frac{\lambda_\alpha + \mathrm{i}u}{\lambda_\alpha - \mathrm{i}u} \right) - \sum_{\beta=\pm 1}^{\pm M} \frac{1}{\mathrm{i}} \ln \frac{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u} \qquad (\mathrm{mod}\ 2\pi). \tag{2.6}$$

The left-hand side of this equation can be transformed as follows,

$$\sum_{l=\pm 1}^{\pm N} \oint_{C_l} \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{1}{\mathrm{i}} \ln \frac{z^2 - 2\mathrm{i}(\lambda_\alpha - \mathrm{i}u)z - 1}{z^2 - 2\mathrm{i}(\lambda_\alpha + \mathrm{i}u)z - 1} \frac{\mathrm{d}}{\mathrm{d}z} \ln P(z) = -\frac{2}{\mathrm{i}} \ln \frac{\lambda - \mathrm{i}u}{\lambda + \mathrm{i}u} - \sum_{l=\pm 1}^{\pm N} \frac{1}{\mathrm{i}} \ln \frac{\tilde{x}_l^2 - 2\mathrm{i}(\lambda_\alpha - \mathrm{i}u)\tilde{x}_l - 1}{\tilde{x}_l^2 - 2\mathrm{i}(\lambda_\alpha + \mathrm{i}u)\tilde{x}_l - 1} - \frac{1}{\mathrm{i}} \ln \eta(\lambda_\alpha; p_1)\eta(\lambda_\alpha; p_L) + \sum_{\beta=\pm 1}^{\pm M} \frac{2}{\mathrm{i}} \ln \frac{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u} \qquad (\mathrm{mod}\ 2\pi) \tag{2.7}$$

where the symbol C_l denotes the contour which encircles $z = x_l$ in the complex plane. In this calculation, we have deformed the contours $\{C_l\}$ $(l = \pm 1, \ldots \pm N)$ to encircle $\{z = \tilde{x}_l\}$ $(l = \pm 1, \ldots \pm N')$, $z = \pm 1$ and the branch cuts of the integrand. Then, we arrive at the following relationships among $\{\tilde{k}_j\}$ $(j = \pm 1 \ldots \pm N')$ and $\{\lambda_\alpha\}$ $(\alpha = \pm 1 \ldots \pm M)$,

$$\prod_{l=\pm 1}^{\pm N'} \frac{\lambda_\alpha - \sin \tilde{k}_l + \mathrm{i}u}{\lambda_\alpha - \sin \tilde{k}_l - \mathrm{i}u} = \check{Y}(\lambda_\alpha; p_1, p_L) \left(-\frac{\lambda_\alpha + \mathrm{i}u}{\lambda_\alpha - \mathrm{i}u} \right)^{-1} \prod_{\beta=\pm 1}^{\pm M} \frac{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u} \tag{2.8}$$

where

$$\check{Y}(\lambda; p_1, p_L) = \begin{cases} \eta(\lambda; p_1)\eta(\lambda; p_L) & \text{for case A} \\ 1 & \text{for case B.} \end{cases} \tag{2.9}$$

Through the above discussions, we have obtained the following relationships among the roots $\{k_j\}$ $(j = 1, \ldots, N)$, $\{\tilde{k}_j\}$ $(j = 1, \ldots, N')$ and $\{\lambda_\alpha\}$ $(\alpha = 1, \ldots, M)$,

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} Z(k_j; p_1, p_L) = \prod_{\beta=1}^{M} \frac{\sin k_j - \lambda_\beta + \mathrm{i}u}{\sin k_j - \lambda_\beta - \mathrm{i}u} \frac{\sin k_j + \lambda_\beta + \mathrm{i}u}{\sin k_j + \lambda_\beta - \mathrm{i}u} \tag{2.10}$$

$$\mathrm{e}^{\mathrm{i}\tilde{k}_j 2(L+1)} Z(\tilde{k}_j; p_1, p_L) = \prod_{\beta=1}^{M} \frac{\sin \tilde{k}_j - \lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j - \lambda_\beta - \mathrm{i}u} \frac{\sin \tilde{k}_j + \lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j + \lambda_\beta - \mathrm{i}u} \tag{2.11}$$

$$\prod_{l=1}^{N} \frac{\lambda_\alpha - \sin k_l + \mathrm{i}u}{\lambda_\alpha - \sin k_l - \mathrm{i}u} \frac{\lambda_\alpha + \sin k_l + \mathrm{i}u}{\lambda_\alpha + \sin k_l - \mathrm{i}u} = Y(\lambda_\alpha; p_1, p_L) \prod_{\substack{\beta=1 \\ (\beta \neq \alpha)}}^{M} \frac{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u} \frac{\lambda_\alpha + \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha + \lambda_\beta - \mathrm{i}2u} \tag{2.12}$$

$$\prod_{l=1}^{N'} \frac{\lambda_\alpha - \sin \tilde{k}_l + \mathrm{i}u}{\lambda_\alpha - \sin \tilde{k}_l - \mathrm{i}u} \frac{\lambda_\alpha + \sin \tilde{k}_l + \mathrm{i}u}{\lambda_\alpha + \sin \tilde{k}_l - \mathrm{i}u} = \check{Y}(\lambda_\alpha; p_1, p_L) \prod_{\substack{\beta=1 \\ (\beta \neq \alpha)}}^{M} \frac{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u} \frac{\lambda_\alpha + \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha + \lambda_\beta - \mathrm{i}2u} \tag{2.13}$$

where we have removed the restrictions for the arguments of the roots in these expressions.

In the following sections, we only discuss the case with $p_1 = p_L = 0$, where the Hubbard model has the $SO(4)$ symmetry. For this case, $Z = Y = \check{Y} = 1$ holds.

3. Low-lying excited energy in the Hubbard open chain at the $SO(4)$ point

3.1. Repulsive Hubbard model

In this section, we derive the energy in the low-lying excited state in the repulsive ($u > 0$) Hubbard open chain with the $SO(4)$ symmetry. Our approach is an extension of Woynarovich's method [11] by which the low-lying excited spectrum in the periodic-boundary case has been discussed.

In our calculations, we use the roots $\{k_j\}$, $\{\tilde{k}_j\}$ and $\{\lambda_\alpha\}$ of equations (2.10)–(2.13) with $Z = Y = \check{Y} = 1$. We assume that we can make the restrictions $0 < \mathrm{Re}\, k_j < \pi$, $0 < \mathrm{Re}\, \tilde{k}_j < \pi$ and $0 < \mathrm{Re}\, \lambda_\alpha$ for the roots of the equations which give the rapidities of independent Bethe ansatz states.

As far as we consider low-lying excited states above the ground state, $2M$ of the possible $L + 2M$ values $\{k_j\}$ and $\{\tilde{k}_{j'}\}$ ($j = 1, \ldots, N,\ j' = 1, \ldots, N'$) can be expected to take the form

$$\sin k_\alpha^{\pm} = \lambda_\alpha \mp \mathrm{i}u + \mathrm{O}(\mathrm{e}^{-\delta L}) \qquad \pm\, \mathrm{Im}\, k_\alpha^{\pm} > 0 (^\exists \delta > 0) \tag{3.1}$$

similarly to the periodic-boundary case [11]. Indeed, we can check that $k_\alpha^{\pm}$ satisfy equations (2.10) and (2.11) (with $Z = 1$). In this section we use the symbol λ_α, to describe only those elements in $\{\lambda_\alpha\}$ which are associated with complex $\tilde{k}_j$'s by the relation (3.1). The other elements of the set $\{\lambda_\alpha\}$, which are associated with complex k_j's, are described by the symbol Λ_α. We assume that the other elements in $\{k_j\}$ ($j = 1, \ldots, N$) and $\{\tilde{k}_j\}$ ($j = 1, \ldots, N'$) are real. Hereafter, we describe only the real elements by the symbols k_j and $\tilde{k}_j$. Therefore, the total number of the real values, k_j's and $\tilde{k}_j$'s, is equal to L.

Then, we can obtain the following equations for the redefined parameters $\{k_j\}$, $\{\tilde{k}_j\}$, $\{\lambda_\alpha\}$ and $\{\Lambda_\alpha\}$,

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} = \prod_\beta \frac{\sin k_j - \lambda_\beta + \mathrm{i}u}{\sin k_j - \lambda_\beta - \mathrm{i}u} \frac{\sin k_j + \lambda_\beta + \mathrm{i}u}{\sin k_j + \lambda_\beta - \mathrm{i}u} \prod_\beta \frac{\sin k_j - \Lambda_\beta + \mathrm{i}u}{\sin k_j - \Lambda_\beta - \mathrm{i}u} \frac{\sin k_j + \Lambda_\beta + \mathrm{i}u}{\sin k_j + \Lambda_\beta - \mathrm{i}u} \tag{3.2}$$

$$\mathrm{e}^{\mathrm{i}\tilde{k}_j 2(L+1)} = \prod_\beta \frac{\sin \tilde{k}_j - \lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j - \lambda_\beta - \mathrm{i}u} \frac{\sin \tilde{k}_j + \lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j + \lambda_\beta - \mathrm{i}u} \prod_\beta \frac{\sin \tilde{k}_j - \Lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j - \Lambda_\beta - \mathrm{i}u} \frac{\sin \tilde{k}_j + \Lambda_\beta + \mathrm{i}u}{\sin \tilde{k}_j + \Lambda_\beta - \mathrm{i}u} \tag{3.3}$$

$$\prod_l \frac{\lambda_\alpha - \sin k_l + \mathrm{i}u}{\lambda_\alpha - \sin k_l - \mathrm{i}u} \frac{\lambda_\alpha + \sin k_l + \mathrm{i}u}{\lambda_\alpha + \sin k_l - \mathrm{i}u} = \prod_{\beta(\neq\alpha)} \frac{\lambda_\alpha - \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha - \lambda_\beta - \mathrm{i}2u} \frac{\lambda_\alpha + \lambda_\beta + \mathrm{i}2u}{\lambda_\alpha + \lambda_\beta - \mathrm{i}2u} \tag{3.4}$$

$$\prod_l \frac{\Lambda_\alpha - \sin \tilde{k}_l + \mathrm{i}u}{\Lambda_\alpha - \sin \tilde{k}_l - \mathrm{i}u} \frac{\Lambda_\alpha + \sin \tilde{k}_l + \mathrm{i}u}{\Lambda_\alpha + \sin \tilde{k}_l - \mathrm{i}u} = \prod_{\beta(\neq\alpha)} \frac{\Lambda_\alpha - \Lambda_\beta + \mathrm{i}2u}{\Lambda_\alpha - \Lambda_\beta - \mathrm{i}2u} \frac{\Lambda_\alpha + \Lambda_\beta + \mathrm{i}2u}{\Lambda_\alpha + \Lambda_\beta - \mathrm{i}2u} \tag{3.5}$$

apart from corrections of order $\mathrm{e}^{-\delta L} (^\exists \delta > 0)$.

In the ground state of the repulsive Hubbard model at the half-filling without the magnetic field, the numbers of the elements $\{k_j\}$, $\{\tilde{k}_j\}$, $\{\lambda_\alpha\}$ and $\{\Lambda_\alpha\}$ are L, 0, $L/2$ and 0, respectively, and all the elements of $\{\lambda_\alpha\}$ are real. We consider the excitation above the ground state.

In accordance with the procedure for the periodic-boundary case [11, 12], we introduce several parameters. By the symbols $\{\lambda_\alpha^{\mathrm{h}}\}$, we describe the positions of the holes in the distribution of the real elements of $\{\lambda_\alpha\}$. We also introduce auxiliary variables $\{\chi_\mu\}$ which generate the complex (i.e. not real) elements of $\{\lambda_\alpha\}$ in the following way,

$$\lambda_\mu = \begin{cases} \chi_\mu \pm \mathrm{i}u & \text{for } |\chi_\mu| < u \\ \chi_\mu + \mathrm{sign}(\mathrm{Im}\,\chi_\mu)\mathrm{i}u & \text{for } |\chi_\mu| > u. \end{cases} \tag{3.6}$$

Since $\{\tilde{k}_j\}$ behaves like the holes in the distribution of $\{k_j\}$, we describe $\{\tilde{k}_j\}$ by the symbols $\{k_j^{\mathrm{h}}\}$. Then, using equations (3.4) and (3.5), we can derive the following equations

$$\prod_{\beta=1}^{H^{\mathrm{s}}+2L^{\mathrm{s}}} \frac{\chi_\mu - \lambda_\beta^{\mathrm{h}} + \mathrm{i}u}{\chi_\mu - \lambda_\beta^{\mathrm{h}} - \mathrm{i}u} \frac{\chi_\mu + \lambda_\beta^{\mathrm{h}} + \mathrm{i}u}{\chi_\mu + \lambda_\beta^{\mathrm{h}} - \mathrm{i}u} = \prod_{\substack{\nu=1 \\ (\nu\neq\mu)}}^{L^{\mathrm{s}}} \frac{\chi_\mu - \chi_\nu + \mathrm{i}2u}{\chi_\mu - \chi_\nu - \mathrm{i}2u} \frac{\chi_\mu + \chi_\nu + \mathrm{i}2u}{\chi_\mu + \chi_\nu - \mathrm{i}2u} \tag{3.7}$$

$$\prod_{l=1}^{H^{\mathrm{c}}+2L^{\mathrm{c}}} \frac{\Lambda_\alpha - \sin k_l^{\mathrm{h}} + \mathrm{i}u}{\Lambda_\alpha - \sin k_l^{\mathrm{h}} - \mathrm{i}u} \frac{\Lambda_\alpha + \sin k_l^{\mathrm{h}} + \mathrm{i}u}{\Lambda_\alpha + \sin k_l^{\mathrm{h}} - \mathrm{i}u} = \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{L^{\mathrm{c}}} \frac{\Lambda_\alpha - \Lambda_\beta + \mathrm{i}2u}{\Lambda_\alpha - \Lambda_\beta - \mathrm{i}2u} \frac{\Lambda_\alpha + \Lambda_\beta + \mathrm{i}2u}{\Lambda_\alpha + \Lambda_\beta - \mathrm{i}2u}. \tag{3.8}$$

Here, the number of the elements $\{\lambda_\alpha^{\mathrm{h}}\}$ is equal to $H^{\mathrm{s}} + 2L^{\mathrm{s}}$, where $H^{\mathrm{s}} \equiv N - 2M$ and L^{s} denotes the number of $\{\chi_\mu\}$, and the number of the elements $\{k_j^{\mathrm{h}}\}$ is equal to $H^{\mathrm{c}} + 2L^{\mathrm{c}}$, where $H^{\mathrm{c}} \equiv L - N$ and L^{c} denotes the number of $\{\Lambda_\alpha\}$. (Refer to the periodic-boundary case [11, 12].) As far as $H^{\mathrm{c}} + 2L^{\mathrm{c}}$ and $H^{\mathrm{s}} + 2L^{\mathrm{s}}$ are much less than L, the positions of the holes $\{k_j^{\mathrm{h}}\}$ and $\{\lambda_\alpha^{\mathrm{h}}\}$ can be recognized as free parameters, similarly to the periodic-boundary case [11, 12]. Once equations (3.7) and (3.8) are solved, the distribution of $\{k_j\}$ and real elements of $\{\lambda_\alpha\}$ can be given by,

$$\begin{aligned} \rho(k) = 2\left(1 + \frac{1}{L}\right)\rho_0(k) + \frac{\cos k}{L} \sum_{\alpha=1}^{L^{\mathrm{c}}} (a_1(\sin k - \Lambda_\alpha) + a_1(\sin k + \Lambda_\alpha)) \\ - \frac{\cos k}{L}\left\{ \sum_{l=1}^{H^{\mathrm{c}}+2L^{\mathrm{c}}} (R(\sin k - \sin k_l^{\mathrm{h}}) + R(\sin k + \sin k_l^{\mathrm{h}})) + R(\sin k) \right\} \\ - \frac{\cos k}{L}\left\{ \sum_{\beta=1}^{H^{\mathrm{s}}+2L^{\mathrm{s}}} (Q(\sin k - \lambda_\beta^{\mathrm{h}}) + Q(\sin k + \lambda_\beta^{\mathrm{h}})) + Q(\sin k) \right\} \end{aligned} \tag{3.9}$$

$$\begin{aligned} \sigma(\lambda) = 2\left(1 + \frac{1}{L}\right)\sigma_0(\lambda) - \frac{1}{L} \sum_{\mu=1}^{L^{\mathrm{s}}} (a_1(\lambda - \chi_\mu) + a_1(\lambda + \chi_\mu)) \\ - \frac{1}{L}\left\{ \sum_{l=1}^{H^{\mathrm{c}}+2L^{\mathrm{c}}} (Q(\lambda - \sin k_l^{\mathrm{h}}) + Q(\lambda + \sin k_l^{\mathrm{h}})) + Q(\lambda) \right\} \\ + \frac{1}{L}\left\{ \sum_{\beta=1}^{H^{\mathrm{s}}+2L^{\mathrm{s}}} (R(\lambda - \lambda_\beta^{\mathrm{h}}) + R(\lambda + \lambda_\beta^{\mathrm{h}})) + R(\lambda) \right\} \end{aligned} \tag{3.10}$$

with

$$\begin{aligned} a_n(\lambda) = \frac{1}{\pi} \frac{nu}{\lambda^2 + (nu)^2} \qquad Q(\lambda) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\omega\lambda}}{2\cosh u\omega} \\ R(\lambda) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\omega\lambda}\mathrm{e}^{-u|\omega|}}{2\cosh u\omega}. \end{aligned} \tag{3.11}$$

Here, we have defined $\rho_0(k)$ and $\sigma_0(\lambda)$ as follows

$$\begin{aligned} \rho_0(k) = \frac{1}{2\pi} + \cos k \int_0^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\cos(\omega \sin k)}{\cosh u\omega} J_0(\omega)\mathrm{e}^{-u\omega} \\ \sigma_0(\lambda) = \int_0^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\cos(\omega\lambda)}{\cosh u\omega} J_0(\omega). \end{aligned} \tag{3.12}$$

Using the distribution functions thus obtained, we can describe the energy as follows

$$\frac{E}{L} = \int_0^\pi \mathrm{d}k\, \epsilon_0(k)\rho(k) + \frac{1}{L}\sum_{\alpha=1}^{L^c}(\epsilon_0(k_\alpha^+) + \epsilon_0(k_\alpha^-)) - \frac{1}{L}\sum_{j=1}^{H^s+2L^s}\epsilon_0(k_j^h) - \frac{1}{2L}(\epsilon_0(0)+\epsilon_0(\pi)) + u + \mathrm{O}\left(\frac{1}{L}\right) \tag{3.13}$$

where

$$\epsilon_0(k) = -2u - 2\cos k \qquad \sin k_\alpha^\pm = \Lambda_\alpha \mp \mathrm{i}u. \tag{3.14}$$

Finally, we obtain the low-lying excited energy of the repulsive Hubbard model with boundaries as follows (up to higher-order corrections of L),

$$E = e_0(u)\times(L+1) + e_1(u) + \sum_{\{k^h\}}\varepsilon_c(k^h) + \sum_{\{\lambda^h\}}\varepsilon_s(\lambda^h) \tag{3.15}$$

with

$$e_0(u) = -u - 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{J_0(\omega)J_1(\omega)}{\cosh u\omega}\mathrm{e}^{-u\omega} \qquad e_1(u) = 1 + \int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{J_1(\omega)}{\cosh u\omega}. \tag{3.16}$$

Here, we have abbreviated $\{k_j^h\}$ and $\{\lambda_\alpha^h\}$ as $\{k^h\}$ and $\{\lambda^h\}$, respectively. The symbols $\varepsilon_c(k)$ and $\varepsilon_s(\lambda)$ are defined by

$$\begin{aligned}\varepsilon_c(k) &= 2u + 2\cos k + 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{\cos(\omega\sin k)}{\cosh u\omega}J_1(\omega)\mathrm{e}^{-u\omega}\\ \varepsilon_s(\lambda) &= 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{\cos(\omega\lambda)}{\cosh u\omega}J_1(\omega).\end{aligned} \tag{3.17}$$

We can recognize the quantities $\varepsilon_c(k)$ and $\varepsilon_s(\lambda)$ as the energies of the holon and the spinon which correspond to the elementary excitations in the charge and the spin sectors, respectively. Those energies take the same forms as the corresponding quantities in the periodic-boundary case [13]. Moreover, the low-lying excited energy in the repulsive Hubbard model under the periodic boundary condition is known to take the form [11, 12]

$$E = e_0(u)\times L + \sum_{\{k^h\}}\varepsilon_c(k^h) + \sum_{\{\lambda^h\}}\varepsilon_s(\lambda^h). \tag{3.18}$$

3.2. Attractive Hubbard model

In this section, we derive the low-lying excitation spectrum of the attractive ($u<0$) Hubbard model with boundaries at the $SO(4)$ point.

As was discussed in section 1, by the transformations

$$c_{j+} \longrightarrow (-1)^j c_{j+}^\dagger \qquad \text{and} \qquad c_{j-}\longrightarrow c_{j-} \tag{3.19}$$

the Hamiltonian $\mathcal{H}(u)$ can be changed into $\mathcal{H}(-u)$ (for $\mathcal{H}^b = 0$). Therefore, we can derive the low-lying spectrum of $\mathcal{H}(u)$ ($u<0$) from that of $\mathcal{H}(|u|)$ without new calculations. (Here, we remark that the number of the fermions and the down spins are equal to $N' \equiv L + 2M - N$ and M in the transformed system $\mathcal{H}(|u|)$, where the corresponding numbers are equal to N and M in the original system $\mathcal{H}(u)$.) Indeed, using the result for the repulsive case (3.15), we can obtain the low-lying excited energy of the attractive Hubbard model with boundaries as follows

$$E = e_0(|u|)\times(L+1) + e_1(|u|) + \sum_{\{k^p\}}\varepsilon_1(k^p) + \sum_{\{\lambda^h\}}\varepsilon_2(\lambda^h). \tag{3.20}$$

Here, the symbols $\varepsilon_1(k)$ and $\varepsilon_2(\lambda)$ are defined by

$$\begin{aligned}\varepsilon_1(k) &= 2|u| - 2\cos k + 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{\cos(\omega\sin k)}{\cosh u\omega}J_1(\omega)\mathrm{e}^{-|u|\omega}\\ \varepsilon_2(\lambda) &= 2\int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{\cos(\omega\lambda)}{\cosh u\omega}J_1(\omega).\end{aligned} \tag{3.21}$$

The energies $\varepsilon_1(k)$ and $\varepsilon_2(\lambda)$ correspond to $\varepsilon_c(k)$ and $\varepsilon_s(\lambda)$, respectively. The parameter k^p in $\varepsilon_1(k^p)$ is introduced by $k^p = \pi - k^h$, where k^h is a free parameter of $\varepsilon_c(k^h)$ in equation (3.15). The quantities $\varepsilon_1(k)$ and $\varepsilon_2(\lambda)$ are expected to describe the energies of quasiparticles, which correspond to the elementary excitations in the spin and the charge sectors, respectively, and take the same forms as those with the periodic boundary condition [13]. Moreover, the low-lying excited energy in the attractive Hubbard model under the periodic boundary condition is known to take the form [11],

$$E = e_0(|u|)\times L + \sum_{\{k^p\}}\varepsilon_1(k^p) + \sum_{\{\lambda^h\}}\varepsilon_2(\lambda^h). \tag{3.22}$$

4. Boundary scattering matrix of the Hubbard open chain at the $SO(4)$ point

4.1. Repulsive Hubbard model

In this section, we derive the boundary scattering matrix for the elementary excitations in the repulsive Hubbard model at the $SO(4)$ point, using Grisaru *et al*'s method [16].

In order to discuss the elementary excitations more directly, we need more detailed forms of the roots for the Bethe ansatz equations than those in section 3.1. Then, we assume that the solutions of the Bethe ansatz equations (1.4) and (1.5) (with $p_1 = p_L = 0$) for $u > 0$ take the following string forms [16]:

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

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

with a real number λ_α^n, apart from a correction of order $\mathrm{e}^{-\delta L}$ ($^\exists\delta > 0$).

(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 $\mathrm{O}(\mathrm{e}^{-\delta L})$ ($^\exists\delta > 0$),

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

with a real number λ'^n_α, and

$$\begin{aligned}
&k_\alpha^1 = \pi - \sin^{-1}(\lambda'^n_\alpha + \mathrm{i}nu) \\
&k_\alpha^2 = \sin^{-1}(\lambda'^n_\alpha + \mathrm{i}(n-2)u) \qquad && k_\alpha^3 = \pi - k_\alpha^2 \\
&k_\alpha^4 = \sin^{-1}(\lambda'^n_\alpha + \mathrm{i}(n-4)u) && k_\alpha^5 = \pi - k_\alpha^4 \\
&\vdots && \vdots \\
&k_\alpha^{2n-2} = \sin^{-1}(\lambda'^n_\alpha - \mathrm{i}(n-2)u) && k_\alpha^{2n-1} = \pi - k_\alpha^{2n-2} \\
&k_\alpha^{2n} = \pi - \sin^{-1}(\lambda'^n_\alpha - \mathrm{i}nu).
\end{aligned}$$

(3) Real k_j's which do not form the above string-type configurations. (Hereafter, we describe only this kind 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.

Within the above string ansatz [16], we can rewrite the Bethe ansatz equation in the following forms within the accuracy of $\mathrm{O}(\mathrm{e}^{-\delta L})(\exists\delta > 0)$

$$\mathrm{e}^{\mathrm{i}k_j 2(L+1)} = \prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m} e\left(\frac{\sin k_j - \lambda_\beta^m}{mu}\right) e\left(\frac{\sin k_j + \lambda_\beta^m}{mu}\right) \times \prod_{m=1}^{\infty}\prod_{\beta=1}^{M'_m} e\left(\frac{\sin k_j - \lambda'^m_\beta}{mu}\right) e\left(\frac{\sin k_j + \lambda'^m_\beta}{mu}\right) \tag{4.1}$$

$$-e\left(\frac{\lambda_\alpha^n}{nu}\right)\prod_{j=1}^{N-2M'} e\left(\frac{\lambda_\alpha^n - \sin k_j}{nu}\right) e\left(\frac{\lambda_\alpha^n + \sin k_j}{nu}\right) = \prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m} E_{nm}\left(\frac{\lambda_\alpha^n - \lambda_\beta^m}{u}\right) E_{nm}\left(\frac{\lambda_\alpha^n + \lambda_\beta^m}{u}\right) \tag{4.2}$$

$$\exp(-\mathrm{i}2(L+1)(\sin^{-1}(\lambda'^n_\alpha + \mathrm{i}nu) + \sin^{-1}(\lambda'^n_\alpha - \mathrm{i}nu))) = -e\left(\frac{\lambda'^n_\alpha}{nu}\right)\prod_{j=1}^{N-2M'} e\left(\frac{\lambda'^n_\alpha - \sin k_j}{nu}\right) e\left(\frac{\lambda'^n_\alpha + \sin k_j}{nu}\right) \times \prod_{m=1}^{\infty}\prod_{\beta=1}^{M'_m} E_{nm}\left(\frac{\lambda'^n_\alpha - \lambda'^m_\beta}{u}\right) E_{nm}\left(\frac{\lambda'^n_\alpha + \lambda'^m_\beta}{u}\right) \tag{4.3}$$

where

$$e(x) = \frac{x+\mathrm{i}}{x-\mathrm{i}} \tag{4.4}$$

$$E_{nm}(x) = \begin{cases} e\left(\frac{x}{|n-m|}\right) e^2\left(\frac{x}{|n-m|+2}\right) e^2\left(\frac{x}{|n-m|+4}\right)\ldots \\ \quad\ldots e^2\left(\frac{x}{n+m-2}\right) e\left(\frac{x}{n+m}\right) & \text{for } n \neq m \\ e^2\left(\frac{x}{2}\right) e^2\left(\frac{x}{4}\right)\ldots e^2\left(\frac{x}{2n-2}\right) e\left(\frac{x}{2n}\right) & \text{for } n = m. \end{cases} \tag{4.5}$$

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

In order to calculate the boundary scattering matrices for the excitations in the charge and the spin sectors, we consider the case with $N = L - 1$, $M_1 = L/2 - 1$, $M_n = 0$ $(n \geqslant 2)$ and $M'_n = 0$ $(n \geqslant 1)$ and introduce one hole in each sector. In this case, we rewrite equations (4.1)–(4.3) to give

$$\frac{I_j}{L} = z_{\mathrm{c}}(k_j) \qquad \frac{J_\alpha}{L} = z_{\mathrm{s}}(\lambda_\alpha) \tag{4.6}$$

where

$$2\pi z_{\mathrm{c}}(k) = 2\left(1+\frac{1}{L}\right)k + \frac{1}{L}\sum_{\beta=1}^{L/2}\left\{\theta\left(\frac{\sin k - \lambda_\beta}{u}\right) + \theta\left(\frac{\sin k + \lambda_\beta}{u}\right)\right\} - \frac{1}{L}\left\{\theta\left(\frac{\sin k - \lambda^{\mathrm{h}}}{u}\right) + \theta\left(\frac{\sin k + \lambda^{\mathrm{h}}}{u}\right)\right\} \tag{4.7}$$

$$2\pi z_{\mathrm{s}}(\lambda) = \frac{1}{L}\theta\left(\frac{\lambda_\alpha}{u}\right) + \frac{1}{L}\sum_{l=1}^{L}\left\{\theta\left(\frac{\lambda - \sin k_l}{u}\right) + \theta\left(\frac{\lambda + \sin k_l}{u}\right)\right\}$$

$$
\begin{aligned}
&-\frac{1}{L}\left\{\theta\left(\frac{\lambda-\sin k^{\mathrm{h}}}{u}\right)+\theta\left(\frac{\lambda+\sin k^{\mathrm{h}}}{u}\right)\right\} \\
&-\frac{1}{L}\sum_{\beta=1}^{L/2}\left\{\theta\left(\frac{\lambda-\lambda_\beta}{2u}\right)+\theta\left(\frac{\lambda+\lambda_\beta}{2u}\right)\right\} \\
&+\frac{1}{L}\left\{\theta\left(\frac{\lambda-\lambda^{\mathrm{h}}}{2u}\right)+\theta\left(\frac{\lambda+\lambda^{\mathrm{h}}}{2u}\right)\right\}
\end{aligned}
\tag{4.8}
$$

with $\theta(x)=2\tan^{-1}x$. Here, $\{I_j\}$ ($j=1,\ldots,L$) and $\{J_\alpha\}$ ($\alpha=1,\ldots,L/2$) take integers and one of $\{I_j\}$ ($\{J_\alpha\}$) corresponds to the hole in the charge (spin) sector. We describe the rapidities corresponding to the holes in the charge and the spin sectors by k^{h} and λ^{h}, respectively. In the present case, one holon exists with the energy $\varepsilon_{\mathrm{c}}(k^{\mathrm{h}})$ and one spinon exists with the energy $\varepsilon_{\mathrm{s}}(\lambda^{\mathrm{h}})$ (see equation (3.15)).

Apart from the contributions of less than $1/L$, we obtain the following forms

$$
\begin{aligned}
2\pi z_{\mathrm{c}}(k) &= -2\left(1+\frac{1}{L}\right)(p_{\mathrm{c}}(k)-p_{\mathrm{c}}(0)) - \frac{1}{L}(\Psi(\sin k-\lambda^{\mathrm{h}})+\Psi(\sin k+\lambda^{\mathrm{h}})+\Psi(\sin k)) \\
&\quad -\frac{1}{L}(\Phi(\sin k-\sin k^{\mathrm{h}})+\Phi(\sin k+\sin k^{\mathrm{h}})+\Phi(\sin k))
\end{aligned}
\tag{4.9}
$$

$$
\begin{aligned}
2\pi z_{\mathrm{s}}(\lambda) &= -2\left(1+\frac{1}{L}\right)(p_{\mathrm{s}}(\lambda)-p_{\mathrm{s}}(0)) - \frac{1}{L}(\Psi(\lambda-\sin k^{\mathrm{h}})+\Psi(\lambda+\sin k^{\mathrm{h}})+\Psi(\lambda)) \\
&\quad +\frac{1}{L}(\Phi(\lambda-\lambda^{\mathrm{h}})+\Phi(\lambda+\lambda^{\mathrm{h}})+\Phi(\lambda)).
\end{aligned}
\tag{4.10}
$$

Here $p_{\mathrm{c}}(k)$ and $p_{\mathrm{s}}(\lambda)$ denote the momenta of the holon and the spinon, which are defined in the corresponding (infinite) periodic system to take the forms [13]

$$
\begin{aligned}
p_{\mathrm{c}}(k) &= \frac{\pi}{2} - k - \int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{\sin(\omega\sin k)}{\cosh u\omega}J_0(\omega)\mathrm{e}^{-u\omega} \\
p_{\mathrm{s}}(\lambda) &= \frac{\pi}{2} - \int_0^\infty \frac{\mathrm{d}\omega}{\omega}\frac{\sin(\omega\lambda)}{\cosh u\omega}J_0(\omega)
\end{aligned}
\tag{4.11}
$$

respectively. Here, we have defined the functions Ψ and Φ as follows

$$
\Psi(\lambda) = \mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\mathrm{e}^{-\mathrm{i}\lambda\omega}}{2\cosh u\omega} \qquad \Phi(\lambda) = \mathrm{i}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\omega}\frac{\mathrm{e}^{-|u\omega|}\mathrm{e}^{-\mathrm{i}\lambda\omega}}{2\cosh u\omega}. \tag{4.12}
$$

Using the functions z_{c} and z_{s} thus obtained, we have

$$
\begin{aligned}
-2\pi z_{\mathrm{c}}(k^{\mathrm{h}})L &= 2(L+1)(p_{\mathrm{c}}(k^{\mathrm{h}})-p_{\mathrm{c}}(0)) + \Psi(\sin k^{\mathrm{h}}-\lambda^{\mathrm{h}}) + \Psi(\sin k^{\mathrm{h}}+\lambda^{\mathrm{h}}) \\
&\quad +\Phi(2\sin k^{\mathrm{h}}) + \Phi(\sin k^{\mathrm{h}}) + \Psi(\sin k^{\mathrm{h}})
\end{aligned}
\tag{4.13}
$$

$$
\begin{aligned}
-2\pi z_{\mathrm{s}}(\lambda^{\mathrm{h}})L &= 2(L+1)(p_{\mathrm{s}}(\lambda^{\mathrm{h}})-p_{\mathrm{s}}(0)) + \Psi(\lambda^{\mathrm{h}}-\sin k^{\mathrm{h}}) + \Psi(\lambda^{\mathrm{h}}+\sin k^{\mathrm{h}}) \\
&\quad -\Phi(2\lambda^{\mathrm{h}}) - \Phi(\lambda^{\mathrm{h}}) + \Psi(\lambda^{\mathrm{h}}).
\end{aligned}
\tag{4.14}
$$

Here, the equalities

$$
2\pi z_{\mathrm{c}}(k^{\mathrm{h}})L = 0 \qquad (\mathrm{mod}\ 2\pi) \qquad 2\pi z_{\mathrm{c}}(\lambda^{\mathrm{h}})L = 0 \qquad (\mathrm{mod}\ 2\pi) \tag{4.15}
$$

hold since evaluation of each of Lz_{c} and Lz_{s} at a root of the Bethe ansatz equations yields an integer by definition.

In accordance with Grisaru *et al*'s method [16], we evaluate the boundary phase shift of the elementary excitations. We focus on the fact that the quantization conditions (see equation (1.13)),

$$2(L+1)p_c(k^h) + \psi_{cs}(\sin k^h - \lambda^h) + \phi_c^L(k^h) + \psi_{cs}(\sin k^h + \lambda^h) + \phi_c^R(k^h) = 0 \pmod{2\pi} \tag{4.16}$$

$$2(L+1)p_s(\lambda^h) + \psi_{cs}(\lambda^h - \sin k^h) + \phi_s^L(\lambda^h) + \psi_{cs}(\lambda^h + \sin k^h) + \phi_s^R(\lambda^h) = 0 \pmod{2\pi}. \tag{4.17}$$

Here, ψ_{cs} denotes the phase shift of the holon–spinon scattering in the bulk, and $\phi_{c(s)}^L$ and $\phi_{c(s)}^R$ denote the phase shift of the holon (spinon) at the left end and right end, respectively.

Comparing equations (4.13)–(4.15) with the quantization conditions (4.16) and (4.17), we can recognize that the relationships

$$\phi_c(\sin k) = \frac{1}{2}(\Phi(2\sin k) + \Phi(\sin k) + \Psi(\sin k)) \tag{4.18}$$

$$\phi_s(\lambda) = -\frac{1}{2}(\Phi(2\lambda) + \Phi(\lambda) - \Psi(\lambda)) \tag{4.19}$$

hold apart from rapidity-independent additive constants, where $\phi_c \equiv \phi_c^L = \phi_c^R$ and $\phi_s \equiv \phi_s^L = \phi_s^R$. Therefore, we can obtain the boundary scattering matrices for the charge and spin sector, as follows

$$K_c(\sin k) = e^{i\phi_c(\sin k)} = \frac{\Gamma\left(1 + i\frac{\mu}{2}\right)\Gamma\left(\frac{1}{4} - i\frac{\mu}{2}\right)}{\Gamma\left(1 - i\frac{\mu}{2}\right)\Gamma\left(\frac{1}{4} + i\frac{\mu}{2}\right)} \qquad \mu = \frac{\sin k}{2u} \tag{4.20}$$

$$K_s(\lambda) = e^{i\phi_s(\lambda)} = \frac{\Gamma\left(1 - i\frac{\mu}{2}\right)\Gamma\left(\frac{3}{4} + i\frac{\mu}{2}\right)}{\Gamma\left(1 + i\frac{\mu}{2}\right)\Gamma\left(\frac{3}{4} - i\frac{\mu}{2}\right)} \qquad \mu = \frac{\lambda}{2u}. \tag{4.21}$$

In these calculations, we can also rederive the scattering matrix (S_{cs}) for the scattering of the holon and the spinon in the bulk [13]. We can identify ψ_{cs} as Ψ to have

$$S_{cs}(\lambda) = e^{i\psi_{cs}(\lambda)} = -i\frac{1 + i\exp\left(\frac{\pi\lambda}{2u}\right)}{1 - i\exp\left(\frac{\pi\lambda}{2u}\right)}. \tag{4.22}$$

4.2. *Attractive Hubbard model*

In this section, we derive the boundary scattering matrices in the attractive Hubbard model at the $SO(4)$ point. For this purpose, we take the same method as that in the previous section.

First, we assume that the solutions of the Bethe ansatz equations (1.4) and (1.5) (with $p_1 = p_L = 0$) for $u < 0$ take the following string forms [16, 13].

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

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

with a real number λ_α^n, apart from a correction of order $e^{-\delta L}(^\exists\delta > 0)$.

(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 $O(e^{-\delta L})(^\exists\delta > 0)$,

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

with a real number λ'^n_α, and

$$\begin{aligned}
&k_\alpha^1 = \sin^{-1}(\lambda'^n_\alpha + in|u|) \\
&k_\alpha^2 = \sin^{-1}(\lambda'^n_\alpha + i(n-2)|u|) \qquad && k_\alpha^3 = \pi - k_\alpha^2 \\
&k_\alpha^4 = \sin^{-1}(\lambda'^n_\alpha + i(n-4)|u|) \qquad && k_\alpha^5 = \pi - k_\alpha^4 \\
&\vdots && \vdots
\end{aligned}$$

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

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

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.

Within the above string ansatz [16, 13], we can rewrite the Bethe ansatz equation in the following forms,

$$\mathrm{e}^{-\mathrm{i}k_j 2(L+1)} = \prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m} e\left(\frac{\sin k_j - \lambda_\beta^m}{m|u|}\right) e\left(\frac{\sin k_j + \lambda_\beta^m}{m|u|}\right)$$
$$\times \prod_{m=1}^{\infty}\prod_{\beta=1}^{M'_m} e\left(\frac{\sin k_j - \lambda'^m_\beta}{m|u|}\right) e\left(\frac{\sin k_j + \lambda'^m_\beta}{m|u|}\right) \tag{4.23}$$

$$-e\left(\frac{\lambda_\alpha^n}{n|u|}\right)\prod_{j=1}^{N-2M'} e\left(\frac{\lambda_\alpha^n - \sin k_j}{n|u|}\right) e\left(\frac{\lambda_\alpha^n + \sin k_j}{n|u|}\right)$$
$$= \prod_{m=1}^{\infty}\prod_{\beta=1}^{M_m} E_{nm}\left(\frac{\lambda_\alpha^n - \lambda_\beta^m}{|u|}\right) E_{nm}\left(\frac{\lambda_\alpha^n + \lambda_\beta^m}{|u|}\right) \tag{4.24}$$

$$\exp(-\mathrm{i}2(L+1)(\sin^{-1}(\lambda'^n_\alpha + \mathrm{i}n|u|) + \sin^{-1}(\lambda'^n_\alpha - \mathrm{i}n|u|)))$$
$$= -e\left(\frac{\lambda'^n_\alpha}{n|u|}\right)\prod_{j=1}^{N-2M'} e\left(\frac{\lambda'^n_\alpha - \sin k_j}{n|u|}\right) e\left(\frac{\lambda'^n_\alpha + \sin k_j}{n|u|}\right)$$
$$\times \prod_{m=1}^{\infty}\prod_{\beta=1}^{M'_m} E_{nm}\left(\frac{\lambda'^n_\alpha - \lambda'^m_\beta}{|u|}\right) E_{nm}\left(\frac{\lambda'^n_\alpha + \lambda'^m_\beta}{|u|}\right) \tag{4.25}$$

apart from a correction of order $\mathrm{e}^{-\delta L}$ ($^\exists\delta > 0$). The ground state corresponds to the case with $N = L$, $M'_1 = L/2$ $M_n = 0$ ($n \geqslant 1$) and $M'_n = 0$ ($n \geqslant 2$).

In order to calculate the boundary scattering matrices for the excitations in the charge and the spin sectors, we consider the case with $N = L - 1$, $M'_1 = L/2 - 1$, $M_n = 0$ ($n \geqslant 1$) and $M'_n = 0$ ($n \geqslant 2$) and introduce one hole in the charge sector and one particle in the spin sector. In this case, we rewrite equations (4.23)–(4.25) to give

$$\frac{I}{L} = z_1(k^{\mathrm{p}}) \qquad \frac{J_\alpha}{L} = z_2(\lambda_\alpha) \tag{4.26}$$

where

$$2\pi z_1(k) = 2\left(1 + \frac{1}{L}\right)k - \frac{1}{L}\sum_{\beta=1}^{L/2}\left\{\theta\left(\frac{\sin k - \lambda_\beta}{|u|}\right) + \theta\left(\frac{\sin k + \lambda_\beta}{|u|}\right)\right\}$$
$$+\frac{1}{L}\left\{\theta\left(\frac{\sin k - \lambda^{\mathrm{h}}}{|u|}\right) + \theta\left(\frac{\sin k + \lambda^{\mathrm{h}}}{|u|}\right)\right\} \tag{4.27}$$
$$2\pi z_2(\lambda) = 2\left(1 + \frac{1}{L}\right)(\sin^{-1}(\lambda + \mathrm{i}|u|) + \sin^{-1}(\lambda - \mathrm{i}|u|)) - \frac{1}{L}\theta\left(\frac{\lambda_\alpha}{|u|}\right)$$
$$-\frac{1}{L}\left\{\theta\left(\frac{\lambda - \sin k^{\mathrm{p}}}{|u|}\right) + \theta\left(\frac{\lambda + \sin k^{\mathrm{p}}}{|u|}\right)\right\}$$

$$-\frac{1}{L}\sum_{\beta=1}^{L/2}\left\{\theta\left(\frac{\lambda-\lambda_\beta}{2|u|}\right)+\theta\left(\frac{\lambda+\lambda_\beta}{2|u|}\right)\right\}$$
$$+\frac{1}{L}\left\{\theta\left(\frac{\lambda-\lambda^{\rm h}}{2|u|}\right)+\theta\left(\frac{\lambda+\lambda^{\rm h}}{2|u|}\right)\right\}. \tag{4.28}$$

Here, I and $\{J_\alpha\}$ ($\alpha = 1,\ldots,L$) take integers. One of $\{J_\alpha\}$ corresponds to the hole in the charge sector and I corresponds to the particle in the spin sector. We describe the rapidities corresponding to the particle in the spin sector and the hole in the charge sector by $k^{\rm p}$ and $\lambda^{\rm h}$, respectively. In the present case, one quasiparticle exists in the spin sector with the energy $\varepsilon_1(k^{\rm p})$ and one quasiparticle exists in the charge sector with the energy $\varepsilon_2(\lambda^{\rm h})$ (see equation (3.20)). Apart from the contributions less than $1/L$, we obtain the following forms

$$2\pi z_1(k) = 2\left(1+\frac{1}{L}\right)(p_1(k)-p_1(0))+\frac{1}{L}(\Psi(\sin k-\lambda^{\rm h})+\Psi(\sin k+\lambda^{\rm h})+\Psi(\sin k))$$
$$+\frac{1}{L}(\Phi(\sin k-\sin k^{\rm p})+\Phi(\sin k+\sin k^{\rm p})+\Phi(\sin k)) \tag{4.29}$$

$$2\pi z_2(\lambda) = -2\left(1+\frac{1}{L}\right)(p_2(\lambda)-p_2(0))-\frac{1}{L}(\Psi(\lambda-\sin k^{\rm p})+\Psi(\lambda+\sin k^{\rm p})+\Psi(\lambda))$$
$$+\frac{1}{L}(\Phi(\lambda-\lambda^{\rm h})+\Phi(\lambda+\lambda^{\rm h})+\Phi(\lambda). \tag{4.30}$$

Here $p_1(k)$ and $p_2(\lambda)$ denote the momenta of the quasiparticle corresponding to the elementary excitations in the spin and the charge sectors, respectively, which are defined by [13]

$$\begin{aligned} p_1(k) &= k-\int_0^\infty\frac{{\rm d}\omega}{\omega}\frac{\sin(\omega\sin k)}{\cosh u\omega}J_0(\omega){\rm e}^{-|u|\omega} \\ p_2(\lambda) &= -\int_0^\infty\frac{{\rm d}\omega}{\omega}\frac{\sin(\omega\lambda)}{\cosh u\omega}J_0(\omega). \end{aligned} \tag{4.31}$$

Therefore, we have

$$2\pi z_1(k^{\rm p})L = 2(L+1)(p_1(k^{\rm p})-p_1(0))+\Psi(\sin k^{\rm p}-\lambda^{\rm h})+\Psi(\sin k^{\rm p}+\lambda^{\rm h})$$
$$+\Phi(2\sin k^{\rm p})+\Phi(\sin k^{\rm p})+\Psi(\sin k^{\rm p}) \tag{4.32}$$

$$-2\pi z_2(\lambda^{\rm h})L = 2(L+1)(p_2(\lambda^{\rm h})-p_2(0))+\Psi(\lambda^{\rm h}-\sin k^{\rm p})+\Psi(\lambda^{\rm h}+\sin k^{\rm p})$$
$$-\Phi(2\lambda^{\rm h})-\Phi(\lambda^{\rm h})+\Psi(\lambda^{\rm h}) \tag{4.33}$$

with

$$2\pi z_1(k^{\rm p})L = 0 \qquad (\text{mod } 2\pi) \qquad 2\pi z_2(\lambda^{\rm h})L = 0 \qquad (\text{mod } 2\pi). \tag{4.34}$$

We take the quantization conditions (see equation (1.13))

$$2(L+1)p_1(k^{\rm p})+\psi_{12}(\sin k^{\rm p}-\lambda^{\rm h})+\phi_1^{\rm L}(\sin k^{\rm p})+\psi_{12}(\sin k^{\rm p}+\lambda^{\rm h})+\phi_1^{\rm R}(\sin k^{\rm p}) = 0$$
$$(\text{mod } 2\pi) \tag{4.35}$$

$$2(L+1)p_2(\lambda^{\rm h})+\psi_{12}(\lambda^{\rm h}-\sin k^{\rm p})+\phi_2^{\rm L}(\lambda^{\rm h})+\psi_{12}(\lambda^{\rm h}+\sin k^{\rm p})+\phi_2^{\rm R}(\lambda^{\rm h}) = 0$$
$$(\text{mod } 2\pi) \tag{4.36}$$

into account to read off the phase shifts from equations (4.32)–(4.34). We have

$$\phi_1(\sin k) = \tfrac{1}{2}(\Phi(2\sin k)+\Phi(\sin k)+\Psi(\sin k)) \tag{4.37}$$

$$\phi_2(\lambda) = -\tfrac{1}{2}(\Phi(2\lambda)+\Phi(\lambda)-\Psi(\lambda)) \tag{4.38}$$

(up to rapidity-independent additive constants), where $\phi_1 \equiv \phi_1^{\mathrm{L}} = \phi_1^{\mathrm{R}}$ and $\phi_2 \equiv \phi_2^{\mathrm{L}} = \phi_2^{\mathrm{R}}$. Therefore, we can obtain the boundary scattering matrices for the spin and charge sector, as follows

$$K_1(\sin k) = \mathrm{e}^{\mathrm{i}\phi_1(\sin k)} = \frac{\Gamma(1+\mathrm{i}\frac{\mu}{2})\Gamma\left(\frac{1}{4}-\mathrm{i}\frac{\mu}{2}\right)}{\Gamma\left(1-\mathrm{i}\frac{\mu}{2}\right)\Gamma\left(\frac{1}{4}+\mathrm{i}\frac{\mu}{2}\right)} \qquad \mu = \frac{\sin k}{2|u|} \tag{4.39}$$

$$K_2(\lambda) = \mathrm{e}^{\mathrm{i}\phi_2(\lambda)} = \frac{\Gamma\left(1-\mathrm{i}\frac{\mu}{2}\right)\Gamma\left(\frac{3}{4}+\mathrm{i}\frac{\mu}{2}\right)}{\Gamma(1+\mathrm{i}\frac{\mu}{2})\Gamma\left(\frac{3}{4}-\mathrm{i}\frac{\mu}{2}\right)} \qquad \mu = \frac{\lambda}{2|u|} \tag{4.40}$$

respectively. In these calculations, we have also rederived the scattering matrix (S_{12}) for the scattering of the quasiparticles corresponding to the charge and the spin sectors in the bulk [13]. We can identify ψ_{12} as Ψ to give

$$S_{12}(\lambda) = \mathrm{e}^{\mathrm{i}\psi_{12}(\lambda)} = -\mathrm{i}\frac{1+\mathrm{i}\exp\left(\frac{\pi\lambda}{2|u|}\right)}{1-\mathrm{i}\exp\left(\frac{\pi\lambda}{2|u|}\right)}. \tag{4.41}$$

5. Summary

In this paper, we have discussed the elementary excitations in the repulsive and the attractive Hubbard models with boundaries at the $SO(4)$ point.

First, we derived the energy in the low-lying excited state where there exist quasiparticles corresponding to the elementary excitations. The results thus obtained take different forms from those of the periodic-boundary case only by a constant term. As is expected, each of the quasiparticles in charge and spin sectors has the same energy as that in the periodic chain.

Next we derived the boundary scattering matrices for the quasiparticles in charge and spin sectors. We found that the boundary scattering matrix for the charge excitation with $u > 0$ takes the same form as that for the spin excitation with $u < 0$, and the matrix for the spin sector with $u > 0$ takes the same form as that for the charge sector with $u < 0$. These relationships may come from the fact that the transformation $c_{j+}^{\dagger} \to (-1)^j c_{j+}$ yields the change $\mathcal{H}(u) \to \mathcal{H}(-u)$ at the $SO(4)$ point and interchanges spin and charge degrees of freedom.

The next step in our investigations may be to determine the boundary scattering matrices for the Hubbard open chain *with* boundary fields. When we obtain the boundary scattering matrices of the Hubbard model *with* or *without* boundary fields, we expect to gain insight into a number of physical properties, similarly to the case of the XXZ open chain [19–21].

For example, we can study the thermodynamics of a field theory describing the low-lying excitations in the Hubbard model. The one-dimensional Hubbard model is recognized as a lattice regularization of the $SU(2)$ Gross–Neveu model, which is an integrable relativistic field theory (see, for example, [22, 23]). A scaling limit yields the integrable field-theoretical model with boundary interactions from the Hubbard open chain. Therefore, by taking an appropriate limit of the boundary scattering matrices of the Hubbard open chain, we may directly derive the matrices describing the boundary scattering [24] in the resulting field theory. Using the scattering matrices thus obtained, we may derive the thermodynamic Bethe ansatz equations for the free energy of the field theory with boundaries. It is known that such a field theory with boundary interactions is closely related to one-dimensional systems with impurities, which have attracted much attention recently (see, for example [20, 21]). Therefore, the boundary scattering matrices may also be useful to investigate impurity problems.

Such physical applications of the scattering matrices will be given in a separate paper.

Note added in proof. After we submitted this paper, Tsuchiya [25] derived boundary scattering matrices for the repulsive Hubbard model with the case-A boundary field. His results correspond to an extension of a part of our results in this paper.

We have also determined boundary scattering matrices for the following four cases [26]:

- repulsive Hubbard model with the case-A boundary field;
- repulsive Hubbard model with the case-B boundary field;
- attractive Hubbard model with the case-A boundary field;
- attractive Hubbard model with the case-B boundary field.

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