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LETTER TO THE EDITOR

Boundary S-matrices for the open Hubbard chain with boundary fields

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Abstract. Using the method introduced by Grisaru *et al*, boundary S-matrices for the physical excitations of the open Hubbard chain with boundary fields are studied. In contrast to the open supersymmetric t-J model, the boundary S-matrix for the charge excitations depend on the boundary fields though the boundary fields do not break the spin-$SU(2)$ symmetry.

Recently, one-dimensional integrable models *with boundaries* have attracted renewed interest. Those models provide relevant information for the boundary effects on the one-dimensional strongly correlated systems. Among others, as for the bulk case, the one-dimensional Hubbard model with open boundary conditions (open Hubbard chain) plays an important role in this field.

In this letter, using the method introduced by Grisaru *et al* [1] (see also [2]), we study the boundary S-matrix for quasiparticles of the open Hubbard chain with boundary fields.

Let us first recall the known facts about the (open) Hubbard chain. The Hamiltonian of the open Hubbard chain with boundary fields is given by $H^{(\pm)} = H^{(\mathrm{open})}_{\mathrm{bulk}} + H^{(\pm)}_{\mathrm{boundary}}$, where

$$H^{(\mathrm{open})}_{\mathrm{bulk}} = -\sum_{j=1}^{L-1}\sum_{\sigma=\uparrow,\downarrow}(\psi^{\dagger}_{j\sigma}\psi_{j+1\sigma} + \psi^{\dagger}_{j+1\sigma}\psi_{j\sigma}) + U\sum_{j=1}^{L}(n_{j\uparrow} - 1/2)(n_{j\downarrow} - 1/2) \tag{1}$$

$$H^{(\pm)}_{\mathrm{boundary}} = -h_1(n_{1\uparrow} \pm n_{1\downarrow}) - h_L(n_{L\uparrow} \pm n_{L\downarrow}). \tag{2}$$

Here U is the coupling constant, h_l is the boundary field at site $l \in \{1, L\}$, $\psi_{j\sigma}$ (respectively $\psi^{\dagger}_{j\sigma}$) denotes the annihilation (respectively the creation) operator of an electron with spin $\sigma \in \{\uparrow, \downarrow\}$ at site $j \in \{1, 2, \ldots, L\}$, and $n_{j\sigma} = \psi^{\dagger}_{j\sigma}\psi_{j\sigma}$ is the number operator.

It is well known that the bulk Hamiltonian $H^{(\mathrm{open})}_{\mathrm{bulk}}$ (on the bipartite lattice, i.e., with even L) possesses an $SO(4) \cong (SU(2) \times SU(2))/\mathbb{Z}_2$ symmetry [3] (see also [4]). That is, together with the ordinary spin-$SU(2)$ symmetry which corresponds to the spin degrees of freedom, $H^{(\mathrm{open})}_{\mathrm{bulk}}$ is also invariant under the action of the so-called η-$SU(2)$ algebra which pertains to the charge degrees of freedom. The boundary Hamiltonian $H^{(+)}_{\mathrm{boundary}}$ (respectively $H^{(-)}_{\mathrm{boundary}}$) breaks the η-$SU(2)$ symmetry (respectively the spin-$SU(2)$ symmetry) down to $U(1)$. Quasiparticle spectra of the attractive Hubbard model and those of the repulsive Hubbard model are related by an interchange of the spin and charge degrees of freedom [5].

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Then, in what follows, we restrict attention to the Hamiltonian $H^{(+)}$ with $U > 0$ (repulsive case).

The open Hubbard chain with boundary fields has been solved by the (coordinate) Bethe ansatz method [6–8]. The Bethe ansatz for this model provides eigenstates of the Hamiltonian $H^{(+)}$ which are parametrized by the two sets of roots ('rapidities') $\{k_j\}_{j=1}^{N}$ and $\{\Lambda_\gamma\}_{\gamma=1}^{M}$. Here N is the number of electrons and M is the number of electrons with down spin. These roots are subject to the (nested) Bethe ansatz equations,

$$e^{i2k_j(L+1)}\beta(k_j,h_1)\beta(k_j,h_L)=\prod_{\delta=1}^{M}\frac{(\Lambda_\delta-\sin k_j-ic/2)(\Lambda_\delta+\sin k_j+ic/2)}{(\Lambda_\delta-\sin k_j+ic/2)(\Lambda_\delta+\sin k_j-ic/2)} \tag{3}$$

$$\prod_{\substack{\delta=1\\ \delta(\neq\gamma)}}^{M}\frac{(\Lambda_\gamma-\Lambda_\delta-ic)(\Lambda_\gamma+\Lambda_\delta-ic)}{(\Lambda_\gamma-\Lambda_\delta+ic)(\Lambda_\gamma+\Lambda_\delta+ic)}=\prod_{j=1}^{N}\frac{(\Lambda_\gamma-\sin k_j-ic/2)(\Lambda_\gamma+\sin k_j-ic/2)}{(\Lambda_\gamma-\sin k_j+ic/2)(\Lambda_\gamma+\sin k_j+ic/2)} \tag{4}$$

where $j=1,\ldots,N$, $\gamma=1,\ldots,M$, and

$$c=U/2 \tag{5}$$

$$\beta(x,h)=\frac{1-h\,e^{-ix}}{1-h\,e^{ix}}. \tag{6}$$

Note that, in this model, the solutions of the Bethe ansatz equations are restricted as $\mathrm{Re}(k_j), \mathrm{Re}(\Lambda_\gamma)\gamma \geqslant 0$ and $k_j, \Lambda_\gamma \neq 0$. The energy of the model is represented as

$$E_N=-2\sum_{j=1}^{N}\cos k_j. \tag{7}$$

Next, we shall briefly review the work of Grisaru *et al* [1]. In [9], Korepin gave a general method for exactly extracting the bulk S-matrix from the Bethe ansatz equations. Then, generalizing this method, Grisaru *et al* proposed the method for determining the boundary S-matrix from the Bethe ansatz equations, and applied this method to the open Heisenberg chain with boundary magnetic fields [1]. Also, using this method, Essler and coworkers [2] calculated the boundary S-matrices for the open supersymmetric t-J model with boundary magnetic fields and those for the open supersymmetric t-J model with an impurity.

An essential ingredient of their method is the following quantization condition [10] for a system of two particles, which has the internal degrees of freedom, with factorized scattering on a line of length $\tilde{L}$,

$$e^{2ip(\theta_1)\tilde{L}}S_{12}(\theta_1-\theta_2)K_1(\theta_1,h_1)S_{12}(\theta_1+\theta_2)K_1(\theta_1,h_L)=1 \tag{8}$$

where θ_j is the rapidity of particle $j=1,2$, and $p(\theta)$ is defined by the *expression* for the momentum of a particle on the corresponding periodic system. Here $S_{12}(\theta_1-\theta_2)$ is the (bulk) S-matrix for the scattering of particles 1 and 2, and $K_1(\theta_1,h)$ is the boundary S-matrix of the scattering for particle 1 off a boundary with boundary field h. Under appropriate conditions on $S_{12}(\theta_1-\theta_2)$ and $K_1(\theta_1,h)$, the equation (8) is equivalent to the following scalar equation (after taking the logarithm):

$$2\tilde{L}p(\theta_1)+(\text{bulk two-body phase shifts})$$
$$+(\text{boundary phase shifts for } h_1 \text{ and } h_L)\equiv 0\,(\mathrm{mod}\,2\pi). \tag{9}$$

Note that, due to the factor $S_{12}(\theta_1+\theta_2)$ in equation (8), the bulk part of the phase shifts contains the phase shifts for the scattering of particle 1 and the mirror image of particle 2.

On the other hand, if the system is Bethe ansatz solvable, it is possible to derive another condition on $p(\theta_1)$ from *the counting function* that is defined by the Bethe ansatz equations. Then, comparing these two conditions, the boundary phase shifts can be evaluated (up to a rapidity independent constant) [1].

We now turn to consider the boundary scatterings of the open Hubbard chain. Since for the open Hubbard chain it is reasonable to consider the length of the system to be $L+1$, then we put $\tilde{L} = L+1$ in the discussions of the scatterings.

In this letter, we only consider the case with the bipartite lattice and the half-filled band, i.e., L even and $N = L$. In this case, the elementary excitations of the periodic Hubbard Hamiltonian transform into the fundamental representations of $SO(4)$ [5, 11]. These elementary excitations are called spinons which carry spin but no charge and holons/antiholons which carry charge but no spin [5, 11, 12]. The excitation spectrum can be determined by the scattering of these elementary excitations. In [5, 11], the bulk S-matrix for the periodic Hubbard chain has been determined by using Korepin's method. This S-matrix has block diagonal form with respect to the scattering of the spin excitations on the spin excitations, the spin excitations on the charge excitations, the charge excitations on the spin excitations and the charge excitations on the charge excitations.

For the open Hubbard chain, the bulk part of the Hamiltonian is also $SO(4)$ invariant. Thus, the elementary excitations are still spinons and holons/antiholons. However, in our choice of Hamiltonian, the η-$SU(2)$ symmetry is broken down to $U(1)$. Thus the total η-spin is not a good quantum number. The boundary S-matrices $K_{\rm spin}(\Lambda, h)$ and $K_{\rm charge}(k, h)$ for spin and charge excitations, respectively, have the following diagonal form, since the Hamiltonian $H^{(+)}$ has $U(1) \times U(1)$ symmetry which corresponds to the preservation of spinon and holon/antiholon numbers:

$$K_{\rm spin}(\Lambda, h) = \begin{pmatrix} \mathcal{A}(\Lambda, h) & 0 \\ 0 & \mathcal{B}(\Lambda, h) \end{pmatrix} \tag{10}$$

$$K_{\rm charge}(k, h) = \begin{pmatrix} \mathcal{C}(k, h) & 0 \\ 0 & \mathcal{D}(k, h) \end{pmatrix}. \tag{11}$$

Since the boundary Hamiltonian (2) does not break the spin-$SU(2)$ symmetry, we expect that the boundary S-matrix for the spin excitations is proportional to the identity matrix, i.e., $\mathcal{A}(\Lambda) = \mathcal{B}(\Lambda)$. In fact, we will confirm this fact. Also we define the corresponding boundary phase shifts by the formulae; $\mathcal{A}(\Lambda, h) = \mathrm{e}^{\mathrm{i}a(\Lambda,h)}$, $\mathcal{B}(\Lambda, h) = \mathrm{e}^{\mathrm{i}b(\Lambda,h)}$, $\mathcal{C}(k, h) = \mathrm{e}^{\mathrm{i}c(k,h)}$ and $\mathcal{D}(k, h) = \mathrm{e}^{\mathrm{i}d(k,h)}$. From the same argument as was given by Grisaru *et al* [1], to determine the above four components, it is sufficient to analyse the highest weight states and the lowest weight states of the spin (respectively charge) excitation with $S = 1$ (respectively $\eta = 1$). Here S (respectively η) denotes the total spin (respectively η-spin) quantum number. Note that although η is not a good quantum number, when there exist boundary fields, we call the states which become $\eta = 1$ states when the boundary fields vanish, $\eta = 1$ states. Note also that, to study the scattering, we can restrict attention to the states near the ground state, i.e., the states which have a microscopic number of holes in the *real* roots.

Let us introduce counting functions for roots $\{k_j\}$ and $\{\Lambda_\gamma\}$ [6–8]. As mentioned above, for later purposes, we need only the real solutions of the Bethe ansatz equations (3) and (4). In this case, taking the logarithm of equations (3) and (4), we have

$$n_j = z_c(k_j) \tag{12}$$

$$I_\gamma = z_s(\Lambda_\gamma) \tag{13}$$

where $z_c(k)$ and $z_s(\Lambda)$ are counting functions for roots $\{k_j\}$ and $\{\Lambda_\gamma\}$, respectively;

$$z_c(k) = \frac{1}{2\pi}\left[2k\tilde{L} + \frac{1}{\mathrm{i}}\ln\beta(k,h_1) + \frac{1}{\mathrm{i}}\ln\beta(k,h_L) - \sum_{\delta=-M}^{M}\Theta(2\sin k - 2\Lambda_\delta) + \Theta(2\sin k)\right] \tag{14}$$

$$z_s(\Lambda) = \frac{1}{2\pi}\left[-\sum_{j=-N}^{N}\Theta(2\Lambda - 2\sin k_j) + \sum_{\delta=-M}^{M}\Theta(\Lambda - \Lambda_\delta) - \Theta(\Lambda)\right] \tag{15}$$

with $\Theta(x) = -2\tan^{-1}(x/c)$. In the above expressions, we have used the 'doubling trick', that is, we have put $\Lambda_{-\delta} = -\Lambda_\delta$, $k_{-j} = -k_j$ and $\Lambda_0, k_0 = 0$. The two sequences of quantum numbers $\{n_j\}_{j=1}^{N}$ and $\{I_\gamma\}_{\gamma=1}^{M}$ (which we call the n-sequence and I-sequence, respectively) take integer values, and label the state of the model. Note that the n_j, which are defined modulo $2\tilde{L}$, take values in the range $0 < n_j \leqslant N$. Also note that, from the formula $|\Theta(x)| \leqslant \pi$, the I_γ are restricted as $0 < I_\gamma \leqslant N - M(= I_{\max})$. For instance, the ground state is characterized by $M = N/2$ (spin singlet) and the configuration $n_j = j$, $I_\gamma = \gamma$.

We shall also introduce the densities of roots and holes. The number of allowed solutions for the Bethe ansatz equations (3) and (4) in the intervals $(k,\ k + \mathrm{d}k)$ and $(\Lambda,\ \Lambda + \mathrm{d}\Lambda)$ are expressed as $\tilde{L}[\rho(k) + \rho^{\mathrm{h}}(k)]\,\mathrm{d}k$ and $\tilde{L}[\sigma(\Lambda) + \sigma^{\mathrm{h}}(\Lambda)]\,\mathrm{d}\Lambda$. Here $\rho(k)$ and $\sigma(\Lambda)$ are the densities of roots (filled solutions), and $\rho^{\mathrm{h}}(k)$ and $\sigma^{\mathrm{h}}(\Lambda)$ are the densities of holes (unfilled solutions). These are determined by the counting functions as follows:

$$\tilde{L}[\rho(k) + \rho^{\mathrm{h}}(k)] = \mathrm{d}z_c(k)/\mathrm{d}k \tag{16}$$

$$\tilde{L}[\sigma(\Lambda) + \sigma^{\mathrm{h}}(\Lambda)] = \mathrm{d}z_s(\Lambda)/\mathrm{d}\Lambda. \tag{17}$$

Conversely, we can determine the counting functions from the integration of the above formulae, if we know the explicit form of $\rho(k)$, $\rho^{\mathrm{h}}(k)$, $\sigma(\Lambda)$ and $\sigma^{\mathrm{h}}(\Lambda)$.

In the thermodynamic limit ($\tilde{L} \to \infty$ with $N/\tilde{L}$ and $M/\tilde{L}$ fixed), we obtain the following formulae:

$$\begin{aligned}\rho(k) + \rho^{\mathrm{h}}(k) = {} & \frac{1}{\pi} + 2\cos k\int_{-B}^{B}\mathrm{d}\Lambda\,\sigma(\Lambda)K(2\sin k - 2\Lambda) \\ & + \frac{1}{\tilde{L}\pi}[\tau(k,h_1) + \tau(k,h_L)] - \frac{2\cos k}{\tilde{L}}K(2\sin k)\end{aligned} \tag{18}$$

$$\sigma(\Lambda) + \sigma^{\mathrm{h}}(\Lambda) = 2\int_{-Q}^{Q}\mathrm{d}k\,\rho(k)K(2\Lambda - 2\sin k) - \int_{-B}^{B}\mathrm{d}\Lambda'\,\sigma(\Lambda')K(\Lambda - \Lambda') + \frac{1}{\tilde{L}}K(\Lambda) \tag{19}$$

where $K(x) = c/[\pi(x^2 + c^2)]$ and $\tau(x,h) = (h\cos x - h^2)/(1 - 2h\cos x + h^2)$. Here the charge and spin pseudo-Fermi-momenta Q and B, respectively, are determined by the conditions

$$\int_{-Q}^{Q}\mathrm{d}k\,\rho(k) = (2N+1)/\tilde{L} \tag{20}$$

$$\int_{-B}^{B}\mathrm{d}\Lambda\,\sigma(\Lambda) = (2M+1)/\tilde{L}. \tag{21}$$

Since we have to determine the densities of order $1/\tilde{L}$, we may expand $\rho(k)$ and $\sigma(\Lambda)$ as

$$\rho(k) = \rho_0(k) + \rho_1(k)/\tilde{L} + \mathrm{O}(1/\tilde{L}^2) \tag{22}$$

$$\sigma(\Lambda) = \sigma_0(\Lambda) + \sigma_1(\Lambda)/\tilde{L} + \mathrm{O}(1/\tilde{L}^2). \tag{23}$$

For example, we can easily derive the ground-state densities $\rho_0^{(g)}(k)$ and $\sigma_0^{(g)}(\Lambda)$ of order $O(\tilde{L}^0)$. In the ground state there are no holes. Also, in the half-filling case, we see $Q = \pi$ and $B = \infty$ for order $O(\tilde{L}^0)$. Then we can solve equations (18) and (19)

$$\rho_0^{(g)}(k) = \frac{1}{\pi} + \frac{\cos k}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}p \, \frac{J_0(p)\, \mathrm{e}^{-\mathrm{i}p\sin k - c|p|/2}}{\cosh(cp/2)} \tag{24}$$

$$\sigma_0^{(g)}(\Lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}p \, \frac{J_0(p)\, \mathrm{e}^{-\mathrm{i}p\Lambda}}{\cosh(cp/2)} \tag{25}$$

where $J_0(p)$ is the zeroth-order Bessel function.

To determine the boundary S-matrices for the open Hubbard chain, we now proceed to study the excitations which are classified by S_z and η_z eigenvalues. Here S_z (respectively η_z) denotes the total z-component of spins (respectively η-spins). We will consider the spin and charge excitations separately.

Spin excitation

We consider the spin excitations. We first investigate the state with $S = 1$, $S_z = 1$. From this excitation, we can determine the component $\mathcal{A}(\Lambda, h)$ of the boundary S-matrix $K_{\mathrm{spin}}(\Lambda, h)$.

The $S = 1, S_z = 1$ state is obtained by $M \to N/2 - 1$ with N fixed. In this case $I_{\max} = N - M = N/2 + 1$. Thus there are two holes $I_1^{\mathrm{h}}, I_2^{\mathrm{h}}$ in the I-sequence, and the n-sequence do not change. We denote the corresponding spin rapidities $\Lambda_\alpha^{\mathrm{h}}$ ($\alpha = 1, 2$), that is, $I_\alpha^{\mathrm{h}} = z_s(\Lambda_\alpha^{\mathrm{h}})$. The hole densities are thus given by

$$\rho^{\mathrm{h}}(k) = 0 \tag{26}$$

$$\sigma^{\mathrm{h}}(\Lambda) = \frac{1}{\tilde{L}}[\delta(\Lambda - \Lambda_1^{\mathrm{h}}) + \delta(\Lambda + \Lambda_1^{\mathrm{h}}) + \delta(\Lambda - \Lambda_2^{\mathrm{h}}) + \delta(\Lambda + \Lambda_2^{\mathrm{h}})]. \tag{27}$$

Then we obtain the integral equations for pairs $(\rho_0(k), \sigma_0(\Lambda))$ and $(\rho_1(k), \sigma_1(\Lambda))$ with integration boundaries Q and B which are defined by equations (20) and (21). Since we determine the densities of order $O(1/\tilde{L})$, the shifts of the integration boundaries from the ground state must be examined of order $O(1/\tilde{L})$. Following [1, 2, 10], we assume that, in the thermodynamic limit, the shifts of the integration boundaries are of order $O(1/\tilde{L}^n)(n \geqslant 2)$ as far as the boundary phase shifts are concerned. Under this assumption, integral equations can be solved. We then obtain $\rho_0(k) = \rho_0^{(g)}(k)$, $\sigma_0(\Lambda) = \sigma_0^{(g)}(\Lambda)$ and

$$\begin{aligned}\rho_1(k) = {} & -\frac{\cos k}{2c}\left\{\frac{1}{\cosh[\pi(\sin k - \Lambda_1^{\mathrm{h}})/c]} + \frac{1}{\cosh[\pi(\sin k + \Lambda_1^{\mathrm{h}})/c]}\right. \\ & \left. + \frac{1}{\cosh[\pi(\sin k - \Lambda_2^{\mathrm{h}})/c]} + \frac{1}{\cosh[\pi(\sin k + \Lambda_2^{\mathrm{h}})/c]}\right\} \\ & + \frac{\cos k}{4\pi^2} \int_{-\infty}^{\infty} \mathrm{d}p \int_{-\pi}^{\pi} \mathrm{d}k' \, [\tau(k', h_1) + \tau(k', h_L)] \frac{\mathrm{e}^{-2\,\mathrm{i}p(\sin k - \sin k') - c|p|}}{\cosh(cp)} \\ & + \frac{\cos k}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}p \frac{\mathrm{e}^{-\mathrm{i}p\sin k - c|p|/2}}{1 + \mathrm{e}^{c|p|}} + \frac{1}{2\pi}[\tau(k, h_1) + \tau(k, h_L)] - 2\cos k K(2\sin k)\end{aligned} \tag{28}$$

$$\begin{aligned}\sigma_1(\Lambda) = {} & -\frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{d}p[\cos(p\Lambda_1^{\mathrm{h}}) + \cos(p\Lambda_2^{\mathrm{h}})] \frac{\mathrm{e}^{-\mathrm{i}p\Lambda}}{1 + \mathrm{e}^{-c|p|}} \\ & + \frac{1}{4\pi c} \int_{-\pi}^{\pi} \mathrm{d}k \frac{\tau(k, h_1) + \tau(k, h_L)}{\cosh[\pi(\sin k - \Lambda)/c]} + \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}p \frac{\mathrm{e}^{-\mathrm{i}p\Lambda - c|p|}}{1 + \mathrm{e}^{-c|p|}}.\end{aligned} \tag{29}$$

From the above formulae, we can obtain the following equation for the counting function $z_s(\Lambda)$ in the thermodynamic limit:

$$-2\pi z_s(\Lambda_1^{\rm h}) = 2\tilde{L}\, p_s(\Lambda_1^{\rm h}) + \mathcal{N}_1(\Lambda_1^{\rm h}) + \mathcal{N}_2(\Lambda_1^{\rm h}, \Lambda_2^{\rm h}) \equiv 0 \,(\mathrm{mod}\, 2\pi) \tag{30}$$

where $p_s(\Lambda_1^{\rm h})$ is defined by the expression for the spinon momentum of the corresponding periodic system [5, 11, 12]:

$$p_s(\Lambda_1^{\rm h}) = -\int_0^\infty \frac{{\rm d}p}{p}\frac{J_0(p)}{\cosh(cp/2)}\sin(p\Lambda_1^{\rm h}). \tag{31}$$

The terms $\mathcal{N}_1(\Lambda_1^{\rm h})$ and $\mathcal{N}_2(\Lambda_1^{\rm h}, \Lambda_2^{\rm h})$ in (30) are given by

$$\mathcal{N}_1(\Lambda_1^{\rm h}) = \gamma(-2\Lambda_1^{\rm h}/c) + \gamma(-\Lambda_1^{\rm h}/c) - \frac{1}{2\pi}\int_{-\pi}^{\pi} {\rm d}k[\tau(k, h_1) + \tau(k, h_L)]$$
$$\times\phi(-{\rm i}(\Lambda_1^{\rm h} - \sin k)/c, 1/4 + {\rm i}(\Lambda_1^{\rm h} - \sin k)/2c) \tag{32}$$

$$\mathcal{N}_2(\Lambda_1^{\rm h}, \Lambda_2^{\rm h}) = \gamma(-(\Lambda_1^{\rm h} - \Lambda_2^{\rm h})/c) + \gamma(-(\Lambda_1^{\rm h} + \Lambda_2^{\rm h})/c) \tag{33}$$

where

$$\phi(x, y) = {\rm i}\int_0^\infty \frac{{\rm d}\omega}{\omega}\frac{(1 - {\rm e}^{-2x\omega})\,{\rm e}^{-2y\omega}}{1 + {\rm e}^{-\omega}}$$
$$= {\rm i}\ln\frac{\Gamma(x + y + 1/2)\Gamma(y)}{\Gamma(x + y)\Gamma(y + 1/2)} \tag{34}$$

$$\gamma(x) = -\phi({\rm i}x, (1 - {\rm i}x)/2)$$
$$= {\rm i}\ln\frac{\Gamma((1 - {\rm i}x)/2)\Gamma(1 + {\rm i}x/2)}{\Gamma((1 + {\rm i}x)/2)\Gamma(1 - {\rm i}x/2)}. \tag{35}$$

We see that $\mathcal{N}_2(\Lambda_1^{\rm h}, \Lambda_2^{\rm h})$ are the bulk phase shifts due to the scatterings of particle 1 and 2, and also particle 1 and the mirror image of particle 2. Similarly, we can conclude that $\mathcal{N}_1(\Lambda_1^{\rm h})$ is the sum of boundary phase shifts for the scattering of particle 1 off boundaries with boundary fields h_1 and h_2. That is, $\mathcal{N}_1(\Lambda) = a(\Lambda, h_1) + a(\Lambda, h_2)$. Therefore we determine $\mathcal{A}(\Lambda, h)$ up to the rapidity independent constant.

To calculate the component $\mathcal{B}(\Lambda, h)$ in equation (10), we next consider the state with $S = 1, S_z = -1$. We find that, for this spin-$SU(2)$ invariant case, the Bethe ansatz equations and energy spectrum of the $S = 1, S_z = -1$ state are trivially the same as those for the $S = 1, S_z = 1$ state. Thus we have $\mathcal{A}(\Lambda, h) = \mathcal{B}(\Lambda, h)$.

Charge excitation

Next we consider the charge excitations. To determine the two components of the boundary S-matrix for the charge excitations, we must consider the $\eta = 1, \eta_z = 1$ state and the $\eta = 1, \eta_z = -1$ state by the Bethe ansatz.

The $\eta = 1, \eta_z = -1$ state is obtained by removing two k's from the ground state, i.e., $N = L - 2$ and $M = N/2$. In this case, we have

$$\sigma^{\rm h}(\Lambda) = 0 \tag{36}$$

$$\rho^{\rm h}(k) = \frac{1}{\tilde{L}}[\delta(k - k_1^{\rm h}) + \delta(k + k_1^{\rm h}) + \delta(k - k_2^{\rm h}) + \delta(k + k_2^{\rm h})]. \tag{37}$$

Similar to the case of the spin excitation, under the assumption for the integration boundaries, we obtain the densities $\sigma_0(\Lambda)$, $\rho_0(k)$, $\sigma_1(\Lambda)$ and $\rho_1(k)$. Results are $\rho_0(k) = \rho_0^{(g)}(k)$, $\sigma_0(\Lambda) =$

$\sigma_0^{(g)}(\Lambda)$ and

$$\rho_1(k) = -\tilde{L}\rho^{\rm h}(k) - \frac{\cos k}{2\pi}\int_{-\infty}^{\infty} {\rm d}p[\cos(p\sin k_1^{\rm h}) + \cos(p\sin k_2^{\rm h})]\frac{{\rm e}^{-c|p|/2}}{\cosh(cp/2)}$$
$$+\frac{\cos k}{8\pi^2}\int_{-\infty}^{\infty}{\rm d}p\int_{-\pi}^{\pi}{\rm d}k'[\tau(k',h_1)+\tau(k',h_L)]\frac{{\rm e}^{-{\rm i}p(\sin k-\sin k')-c|p|}}{\cosh(cp/2)}$$
$$+\frac{\cos k}{2\pi}\int_{-\infty}^{\infty}{\rm d}p\frac{{\rm e}^{-{\rm i}p\sin k-c|p|/2}}{1+{\rm e}^{c|p|}} + \frac{1}{2\pi}[\tau(k,h_1)+\tau(k,h_L)] \tag{38}$$

$$\sigma_1(\Lambda) = -\frac{1}{2c}\left\{\frac{1}{\cosh[\pi(\Lambda-\sin k_1^{\rm h})/c]} + \frac{1}{\cosh[\pi(\Lambda+\sin k_1^{\rm h})/c]}\right.$$
$$\left.+\frac{1}{\cosh[\pi(\Lambda-\sin k_2^{\rm h})/c]} + \frac{1}{\cosh[\pi(\Lambda+\sin k_2^{\rm h})/c]}\right\}$$
$$+\frac{1}{4\pi c}\int_{-\pi}^{\pi}{\rm d}k\frac{\tau(k,h_1)+\tau(k,h_L)}{\cosh[\pi(\sin k-\Lambda)/c]} + \frac{1}{2\pi}\int_{-\infty}^{\infty}{\rm d}p\frac{{\rm e}^{-{\rm i}p\Lambda}}{1+{\rm e}^{c|p|}}. \tag{39}$$

Also, we have the counting function in the thermodynamic limit

$$-2\pi z_c(k_1^{\rm h}) = 2\tilde{L}p_c^{\eta_z=-1}(k_1^{\rm h}) + \mathcal{M}_1(k_1^{\rm h}) + \mathcal{M}_2(k_1^{\rm h},k_2^{\rm h}) \equiv 0\ (\mathrm{mod}\,2\pi) \tag{40}$$

where $p_c^{\eta_z=-1}(k_1^{\rm h})$ is the quasiparticle momentum of the corresponding periodic system [5, 11, 12]

$$p_c^{\eta_z=-1}(k_1^{\rm h}) = -k_1^{\rm h} - \int_0^{\infty}\frac{{\rm d}p}{p}\frac{J_0(p)\,{\rm e}^{-cp/2}}{\cosh(cp/2)}\sin(p\sin k_1^{\rm h}) \tag{41}$$

and

$$\mathcal{M}_1(k_1^{\rm h}) = \gamma(-2\sin k_1^{\rm h}/c) - 2k_1^{\rm h} - \frac{1}{\rm i}[\ln\beta(k_1^{\rm h},h_1)+\ln\beta(k_1^{\rm h},h_L)]$$
$$-\phi({\rm i}\sin k_1^{\rm h}/c, 3/4-{\rm i}\sin k_1^{\rm h}/c) - \Theta(2\sin k_1^{\rm h})$$
$$-\frac{1}{2\pi}\int_{-\pi}^{\pi}{\rm d}k'[\tau(k',h_1)+\tau(k',h_L)]\gamma(-(\sin k'-\sin k_1^{\rm h})/c) \tag{42}$$

$$\mathcal{M}_2(k_1^{\rm h},k_2^{\rm h}) = \gamma(-(\sin k_1^{\rm h}-\sin k_2^{\rm h})/c) + \gamma(-(\sin k_1^{\rm h}+\sin k_2^{\rm h})/c). \tag{43}$$

Then, we can determine the component $\mathcal{D}(k,h)$ from $\mathcal{M}_1(k_1^{\rm h})$.

Finally, we have to determine the remaining component $\mathcal{C}(k,h)$ in (11). Let us study the $\eta=1$, $\eta_z=1$ state to determine $\mathcal{C}(k,h)$. Since the $\eta=1$, $\eta_z=1$ state is not the regular Bethe ansatz state [4], we must take the completely-filled state $|\Omega\rangle = \prod_{j=1}^{L}\psi_{j\uparrow}^{\dagger}\psi_{j\downarrow}^{\dagger}|0\rangle$ as the Bethe ansatz vacuum. The Bethe ansatz state with $2L-N$ electrons is thus given as

$$|\Phi_N\rangle = \sum_{\sigma_1,\ldots,\sigma_N\in\{\uparrow,\downarrow\}}\Phi_{\sigma_1,\ldots,\sigma_N}(n_1,\ldots,n_N)\prod_{i=1}^{N}\psi_{n_i\sigma_i}|\Omega\rangle \tag{44}$$

where the n_i denotes the location of electrons on the chain. It is easy to see that the eigenvalue of the Hamiltonian $H^{(+)}$ for this state is given by $E_N' = -E_N$, and the Bethe ansatz equations are obtained by taking $c\to -c$ in equations (3) and (4). Then the problem reduces to finding the eigenstates of the attractive Hubbard model with the eigenvalues which are given by changing those signs from the corresponding eigenvalues for the repulsive case. That is, the ground-state configuration of rapidities for our model is identical to the highest energy configuration of rapidities for the attractive case. This is the configuration that all rapidities are real and $N=L$, $M=N/2$ [13]. Therefore, the $\eta=1$, $\eta_z=1$ state is obtained

by removing two k's from the ground-state configuration. Repeating the calculation similar to the case of the $\eta = 1, \eta_z = -1$ state, we have

$$2\pi z_c(k_1^{\rm h}) = 2\tilde{L}\, p_c^{\eta_z=1}(k_1^{\rm h}) + \mathcal{M}_1'(k_1^{\rm h}) + \mathcal{M}_2'(k_1^{\rm h}, k_2^{\rm h}) \equiv 0 \,(\mathrm{mod}\, 2\pi) \tag{45}$$

where $p_c^{\eta_z=1}(k_1^{\rm h})$ is the quasiparticle momentum (note that $p_c^{\eta_z=1}$ is different to $p_c^{\eta_z=-1}$)

$$p_c^{\eta_z=1}(k_1^{\rm h}) = k_1^{\rm h} - \int_0^\infty \frac{{\rm d}p}{p} \frac{J_0(p)\,{\rm e}^{-cp/2}}{\cosh(cp/2)} \sin(p \sin k_1^{\rm h}) \tag{46}$$

and

$$\begin{aligned}\mathcal{M}_1'(k_1^{\rm h}) = {} & \gamma(-2\sin k_1^{\rm h}/c) + 2k_1^{\rm h} + \frac{1}{\rm i}[\ln\beta(k_1^{\rm h}, h_1) + \ln\beta(k_1^{\rm h}, h_L)] \\ & -\phi({\rm i}\sin k_1^{\rm h}/c, 3/4 - {\rm i}\sin k_1^{\rm h}/2c) - \Theta(2\sin k_1^{\rm h}) \\ & -\frac{1}{2\pi}\int_{-\pi}^{\pi} {\rm d}k'[\tau(k', h_1) + \tau(k', h_L)]\gamma(-(\sin k' - \sin k_1^{\rm h})/c)\end{aligned} \tag{47}$$

$$\mathcal{M}_2'(k_1^{\rm h}, k_2^{\rm h}) = \gamma(-(\sin k_1^{\rm h} - \sin k_2^{\rm h})/c) + \gamma(-(\sin k_1^{\rm h} + \sin k_2^{\rm h})/c). \tag{48}$$

As for the case of the $\eta = 1, \eta_z = -1$ state, we obtain the component $\mathcal{C}(k, h)$ from $\mathcal{M}_1(k_1^{\rm h})$.

Boundary S-matrices

Now let us summarize the results. Up to rapidity-independent phase factors, the resulting boundary S-matrices are expressed as

$$K_{\rm spin}(\Lambda, h) = {\rm e}^{\mathcal{X}_s(\Lambda,h)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{49}$$

$$K_{\rm charge}(k, h) = {\rm e}^{\mathcal{X}_c(k,h)} \begin{pmatrix} \beta(k, h) & 0 \\ 0 & \beta(k, h)^{-1} \end{pmatrix} \tag{50}$$

where

$$\begin{aligned}2\mathcal{X}_s(\Lambda, h) = {} & \gamma(-2\Lambda/c) + \gamma(-\Lambda/c) \\ & -\frac{1}{\pi}\int_{-\pi}^{\pi} {\rm d}k\, \tau(k, h)\phi(-{\rm i}(\Lambda - \sin k)/c, 1/4 + {\rm i}(\Lambda - \sin k)/2c)\end{aligned} \tag{51}$$

$$\begin{aligned}2\mathcal{X}_c(k, h) = {} & \gamma(-2\sin k/c) - \phi({\rm i}\sin k/c, 3/4 - {\rm i}\sin k/2c) - \Theta(2\sin k) \\ & -\frac{1}{\pi}\int_{-\pi}^{\pi} {\rm d}k'\, \tau(k', h)\gamma(-(\sin k' - \sin k)/c).\end{aligned} \tag{52}$$

It is worth noting that, in contrast to the case of the open supersymmetric t-J model [2], the boundary S-matrix for the spin excitations depends on the boundary field although the boundary field does not break the spin-$SU(2)$ symmetry.

If the boundary fields vanish, the boundary S-matix of the charge excitations becomes proportional to the identity matrix as expected. The bulk S-matrices for the Hubbard chain [5, 11] and the supersymmetric t-J model [2] have the same form as that for the XXX chain. However, the boundary S-matrix for the open Hubbard chain has different form with the one for the open XXX model. Full details and applications of our results will be published elsewhere.

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