Exact solutions of 1-D Hubbard model with open boundary conditions and the conformal dimensions under boundary magnetic fields

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Abstract

The Bethe ansatz equations of the 1-D Hubbard model under open boundary conditions are systematically derived by diagonalizing the inhomogeneous transfer matrix of the XXX model with open boundaries. Through the finite-size correction, we obtain the energy spectrum of the open chain and discuss the effects of boundary magnetic fields applied only at the edges of the chain. Several physical implications of the finite-size spectrum are discussed from the viewpoint of the boundary conformal field theories (BCFT); the conformal dimension of the spin excitation is quite sensitive to the boundary magnetic fields, and this sensitivity can be explained in terms of the \( \pi/2 \)-phase shift of the BCFT. For several limiting cases such as for the half-filling case, the conformal dimensions are explicitly calculated.

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1 Introduction

In the study of the conformal properties of the critical 2-dimensional classical systems and 1-dimensional quantum models, the analysis of the finite-size correction of the energy spectrum has been proved to be very fruitful. The method can be applied not only to the models under the periodic boundary condition but also to those of the different boundary conditions. From the viewpoint of the boundary conformal field theories (BCFT) many important properties of quantum systems under different boundary conditions have been discussed, such as the Kondo problem and the impurity effects. They are also discussed by the Bethe ansatz. Under the open-boundary condition, the finite-size correction of the energy spectrum consistent with the BCFT has the following expression

\[ E = L e_{\infty} + e_{\text{sur}} + \frac{\pi v_f}{L} \left( -\frac{c}{24} + \Delta_p \right) \]  

where \( c, \Delta_p, v_f, L, e_{\infty}, \) and \( e_{\text{sur}} \) are the central charge, the conformal dimension, the Fermi velocity, the system size, the ground-state energy density of the infinite system, and the surface energy, respectively.

The 1-dimensional Hubbard model is one of the most important solvable models in condensed matter physics. It describes interacting electrons on the 1-dimensional lattice. The low-excitation spectrum depends on the parameters of the model such as the Coulomb repulsion \( U \), the band-width \( t \), the chemical potential \( \mu \), and the magnetic field \( h \); for instance, the model describes the metal-insulator transition at the half-filling band where the charge excitation has the gap.

In this paper, we derive exact solutions of the Hubbard model under general open-boundary conditions, diagonalizing the Hamiltonian partially by the algebraic Bethe ansatz of the open-boundary XXX model. Applying the method of the finite-size correction we obtain the low-excitation spectrum of the open Hubbard Hamiltonian for several regions of the model-parameters. We find that the finite-size spectrum and related critical exponents are different from those of the periodic boundary condition. From the viewpoint of the BCFT, we derive several physical consequences of the low-energy spectrum, such as the \( \pi/2 \)-phase shift due to the magnetic impurity at the boundary, the Fermi-edge singularity in the X-ray absorption spectrum, and a two-impurity problem, etc. It should be remarked that the effect of boundary conditions is closely related to the impurity effect. Thus, we study exactly some aspects of the boundary or impurity effect in strongly correlated electrons in 1D.

There are several motivations for the study of the present paper. The effect of boundary conditions in 1 dim. interacting electrons should be important in condensed matter physics, in particular, in the mesoscopic systems such as the quantum wire. We note that the low-energy properties of 1D electrons are often described by the
Tomonaga-Luttinger liquid. In fact, there are strong motivations for the study of the impurity effect in 1D electrons or the Tomonaga-Luttinger liquid. [16, 17, 6, 7] With respect to the electron interaction, however, it seems that it has been investigated only through some perturbative arguments. Thus it is interesting to discuss the effect of boundary conditions by studying the exactly solvable models in 1D with the bulk electron interaction.

From the viewpoint of the BCFT, the Bethe ansatz study of the Hubbard model under the general open-boundary conditions could also be interesting. The Kondo problem has been discussed [1] by mapping the 3-D Hamiltonian into the effective 1-D system where the Coulomb interaction is active only at the boundary. For the open-boundary Hubbard model in 1D, the spectrum should depend on both the boundary condition and the bulk interaction among electrons. From the standard BCFT approach it would not be easy to make an exact connection of the model-parameters to the spectrum so that we can see how the spectrum should depend on the bulk interaction among electrons. From the Bethe ansatz solutions, however, we can derive a precise connection of the parameters to the low-excitation spectrum. Then we shall see that the expressions of the spectra derived by the Bethe ansatz are very close to those expected by the BCFT.

Let us now discuss how to diagonalize the Hamiltonian of the 1-D Hubbard model under the general open-boundary conditions. After Sklyanin’s pioneering work on the reflection equations [18], there have been many works on integrable models under open-boundary conditions. Making use of the knowledge accumulated in the progress we can study integrable models under general boundary conditions; the Bethe ansatz equations and the eigenvalues of the transfer matrix under the most general conditions can be systematically derived through the algebraic Bethe ansatz method based on the reflection equations. For the open-boundary Hubbard model, the expressions of the Bethe ansatz equations can be derived from the reflection equations of the XXZ model.

For the 1-D Hubbard model, we introduce the Hamiltonian under the general open-boundary conditions in the following

\[ H = -t \sum_{j=1}^{L-1} \sum_{\sigma=\uparrow, \downarrow} \left( c_{j+1 \sigma}^\dagger c_{j \sigma} + c_{j \sigma}^\dagger c_{j+1 \sigma} \right) + U \sum_{j=1}^{L} n_{j \uparrow} n_{j \downarrow} + \mu \sum_{j=1}^{L} (n_{j \uparrow} + n_{j \downarrow}) \]

\[ -\frac{\hbar}{2} \sum_{j=1}^{L} (n_{j \uparrow} - n_{j \downarrow}) + \sum_{\sigma=\uparrow, \downarrow} (p_{1 \sigma} n_{1 \sigma} + p_{L \sigma} n_{L \sigma}) \]

(1.2)

where \( p_{1 \sigma} \) and \( p_{L \sigma} \) (for \( \sigma = \uparrow, \downarrow \)) are the free parameters describing the boundary external fields. We find that the system is integrable under the condition \( p_{1 \uparrow} = \pm p_{1 \downarrow} \) and \( p_{L \uparrow} = \pm p_{L \downarrow} \), i.e., there are four kinds of boundary conditions which are consistent with the integrability. In fact, for the special case of \( p_{1 \uparrow} = p_{1 \downarrow} = p_{L \uparrow} = p_{L \downarrow} = p \), the solution of the model was discussed in [19] and [20]. Hereafter we shall assume \( t = 1 \).
The content of the paper is given in the following. In §2 we shall derive the Bethe ansatz equations for the Hamiltonian (1.2) in two steps; we first diagonalize the particle degrees of freedom (“charge part”) of the Hamiltonian by the coordinate Bethe ansatz method and then the spin degrees of freedom (“spin part”) by the algebraic Bethe ansatz method of the inhomogeneous XXZ model under the open boundary condition, which is based on the reflection equations. In §3 we calculate the finite-size corrections of the energy spectrum of the model under the general boundary terms. In §4 we discuss the spectrum from the viewpoint of BCFT. The conformal dimensions of charge and spin excitations are calculated for the different boundary cases. We show that under zero magnetic field ($h = 0$) the conformal dimension of the spin sector takes distinct values for the different cases of the boundary magnetic fields. We derive some physical implications of the finite-size spectrum from the BCFT viewpoint. In particular, the boundary magnetic fields can be considered as some magnetic impurities of the $\pi/2$-phase shift. We discuss the Fermi-edge singularity and a two-impurity problem, and then the finite-size spectrum under a strong magnetic field. In §5 we calculate the conformal dimensions of the spin excitation for the half-filling case and under the nonzero uniform magnetic field. They depend on both the magnetic field and the boundary magnetic fields. In §6 we give some concluding remarks.

2 Derivation of the Bethe ansatz equations

We shall briefly derive the Bethe ansatz equations for the Hubbard model with open boundaries. The eigenstate with $N$ electrons and $M$ down-spin electrons can be written as

$$\Psi_{NM} = \sum f(x_1, \cdots, x_N) c_{x_1 \sigma_1}^\dagger \cdots c_{x_N \sigma_N}^\dagger |\text{vac}\rangle$$

(2.1)

Here, the $x_j$ denotes the position of electrons, $\sigma_j$ the spin direction. We note that the wave function $f$ also depends on the spin variables $\{\sigma_1, \cdots, \sigma_N\}$. For notational simplicity, we do not write it explicitly. In the region $x_{q_1} \leq \cdots \leq x_{q_N}$, the wave function $f$ takes the form

$$f(x_1, \cdots, x_N) = \sum_P \epsilon_P A_{\sigma_1 \cdots \sigma_N} (k_{p_1}, \cdots, k_{p_N}) \exp\{i \sum_{j=1}^N k_{p_j} x_{q_j}\} \theta(x_{q_1} \leq x_{q_1} \cdots \leq x_{q_N})$$

(2.2)

where the $Q$ runs over $S_N$, the permutation group of $N$ particles, and $P$ over all the permutations and the ways of negations of $k'$s. There are $N! \times 2^N$ possibilities for $P$, while $N!$ for $Q$. We recall that $\epsilon_P$ denotes the sign of $P$. If the permutation is even, $P$ makes $\epsilon_P = -1$ for odd number of $k$’s negative and $\epsilon_P = 1$ for even number of $k$’s negative. The amplitudes satisfy (see Appendix A)
\[ A_{\sigma_1, \ldots, \sigma_N}(k_{p_1}, \ldots, k_{p_N}) = \sum_{\sigma'_1, \ldots, \sigma'_N} \{U(k_{p_1})X_{12}X_{13} \cdots X_{1N}V(k_{p_1}) \}
\]

\[ X_{N1} \cdots X_{21} \}^{\sigma'_1, \ldots, \sigma'_N} A_{\sigma'_1, \ldots, \sigma'_N}(k_{p_1}, \ldots, k_{p_N}), \quad (2.3) \]

where

\[ X_{ij} = \frac{iU/2}{\sin k_{p_i} - \sin k_{p_j} + iU/2} P_{\sigma_i, \sigma_j} + \frac{\sin k_{p_i} - \sin k_{p_j}}{\sin k_{p_i} - \sin k_{p_j} + iU/2} I, \]

\[ X_{ij} = \frac{iU/2}{-\sin k_{p_i} - \sin k_{p_j} + iU/2} P_{\sigma_i, \sigma_j} + \frac{-\sin k_{p_i} - \sin k_{p_j}}{-\sin k_{p_i} - \sin k_{p_j} + iU/2} I, \]

\[ U(k_{p_j}) = \text{diag} \left( \frac{\alpha_\uparrow(k)}{\alpha_\downarrow(-k)}, \frac{\alpha_\downarrow(k)}{\alpha_\uparrow(-k)} \right), \]

\[ V(k_{p_j}) = \text{diag} \left( \frac{\beta_\uparrow(k)}{\beta_\downarrow(-k)}, \frac{\beta_\downarrow(k)}{\beta_\uparrow(-k)} \right). \quad (2.4) \]

Here \( P_{\sigma_i, \sigma_j} \) denotes the permutation operator acting on the spin variables \( \sigma_i \)'s. The symbols \( \alpha_\sigma(k), \beta_\sigma(k) \) are given by equation (A.4).

Let us diagonalize the equation (2.3). We want to determine the matrices \( U \)'s and \( V \)'s so that the system is integrable, i.e., the equation (2.3) can be diagonalized for arbitrary sets of values of \( k \)'s. The key observation is that the form of the equation (2.3) is similar to that of the transfer matrix of the inhomogeneous XXX model under the open boundary condition which was discussed by Sklyanin [18]. Applying the results given by Sklyanin, we obtain the final results (see Appendix A)

\[ E = N\mu - \frac{1}{2}h(N - 2M) - 2 \sum_{j=1}^{N} \cos k_j \quad (2.5) \]

where the parameters \( k_j \) are given by

\[ \frac{(e^{-ik_j}p_{1\uparrow} + 1)(e^{ik_j} + p_{L\uparrow})}{(e^{ik_j}p_{1\uparrow} + 1)(e^{-ik_j} + p_{L\uparrow})} e^{i2k_jL} \]

\[ = \prod_{m=1}^{M} \frac{(\sin k_j - v_m + iU/4)(\sin k_j + v_m + iU/4)}{(\sin k_j - v_m - iU/4)(\sin k_j + v_m - iU/4)}. \quad (2.6) \]
\[
\frac{(\zeta_+ - v_m - iU/4)(\zeta_- - v_m - iU/4)}{(\zeta_+ + v_m - iU/4)(\zeta_- + v_m - iU/4)} \prod_{m \neq n}^M \frac{(v_m - v_n + iU/2)(v_m + v_n + iU/2)}{(v_m - v_n - iU/2)(v_m + v_n - iU/2)}
\]

\[
= \prod_{j=1}^N \frac{(v_m - \sin k_j + iU/4)(v_m + \sin k_j + iU/4)}{(v_m - \sin k_j - iU/4)(v_m + \sin k_j - iU/4)}
\]

(2.7)

where

\[
\zeta_+ = \begin{cases} 
\infty & \text{for } p_{1\uparrow} = p_{1\downarrow} \\
\frac{1 - p_{1\uparrow}^2}{2i p_{1\uparrow}} & \text{for } p_{1\uparrow} = -p_{1\downarrow}
\end{cases}, \quad \zeta_- = \begin{cases} 
\infty & \text{for } p_{L\uparrow} = p_{L\downarrow} \\
\frac{1 - p_{L\uparrow}^2}{2i p_{L\uparrow}} & \text{for } p_{L\uparrow} = -p_{L\downarrow}
\end{cases}
\]

(2.8)

We give a remark. It has been shown in Ref. [21] that for the \(\delta\)-interaction problem in 1-dimension under the periodic boundary condition, the Bethe ansatz equations [22] for the \(N\)-particle system can be recovered from those of the inhomogeneous 6 vertex model and by using the expression of the eigenvalues of the inhomogeneous transfer matrix. [21]

From equation (2.8), we see that the system is integrable under the conditions \(p_{1\sigma} = \pm p_{1-\sigma}\) and \(p_{L\sigma} = \pm p_{L-\sigma}\). We should recall that if the boundary condition is \(p_{1\uparrow} = p_{1\downarrow} = p_{L\uparrow} = p_{L\downarrow} = p\) and \(h = 0\), the Bethe ansatz equations and the energy are reduced to those in reference [20]. In Ref. [19] the Bethe ansatz equations of the 1D Hubbard model under open-boundary condition are discussed for the case of the zero boundary-chemical potential \((p_{1\uparrow} = p_{1\downarrow} = p_{L\uparrow} = p_{L\downarrow} = 0)\). We note that the derivation of Bethe ansatz equations and the energy spectrum for the general boundary conditions is not trivial.

### 3 Finite-size correction of the energy spectrum

Let us discuss the low-excitation spectrum of the open-boundary Hubbard model under the most general boundary conditions; to the Hamiltonian (1.2) under the four different open-boundary conditions we apply the method of the finite-size correction. For the periodic boundary condition it was discussed in Ref. [3]. We shall see, however, that the spectrum of the open-boundary case has several different points from that of the periodic one. The results in this section also generalize Ref. [20], so that we can discuss the boundary effects from the viewpoint of the boundary conformal field theories, as we shall see in §4.

We first take the logarithm of the Bethe ansatz equations (2.6) and (2.7). Then we

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1. We would like to thank Prof. Y. Akutsu for his comment on the Ref. [21].
have

$$2Lk_j = 2\pi I_j - \phi(k_j) - \psi(k_j)$$

$$0 = 2\pi J_m - \Gamma_+ (v_m) - \Gamma_-(v_m)$$

$$- \sum_{m=1}^{M} \left( 2 \tan^{-1} \left( \frac{\sin k_j - v_m}{U/4} \right) + \tan^{-1} \left( \frac{\sin k_j + v_m}{U/4} \right) \right)$$

$$(I_j \in \mathbb{Z})$$

$$(3.1)$$

$$- \sum_{j=1}^{N} \left( 2 \tan^{-1} \left( \frac{v_m - \sin k_j}{U/4} \right) + \tan^{-1} \left( \frac{v_m + \sin k_j}{U/4} \right) \right)$$

$$(J_m \in \mathbb{Z})$$

$$+ \sum_{n \neq m}^{M} \left( 2 \tan^{-1} \left( \frac{v_m - v_n}{U/2} \right) + \tan^{-1} \left( \frac{v_m + v_n}{U/2} \right) \right)$$

$$(3.2)$$

where $I_j$ and $J_m$ are integers and

$$\phi(k_j) = \frac{1}{i} \log \frac{1 + p_{1+} e^{-ik_j}}{1 + p_{1+} e^{ik_j}}$$

$$\psi(k_j) = \frac{1}{i} \log \frac{p_{L+} + e^{ik_j}}{p_{L+} + e^{-ik_j}}$$

$$\Gamma_{\pm}(v) = \frac{1}{i} \log \frac{U/4 + i(\zeta_{\pm} - v)}{U/4 + i(\zeta_{\pm} + v)}$$

It should be emphasized that for $I_j$ and $J_m$ there is no such selection rule as in the periodic case.

Let $\rho_L$ denote the vector $(\rho^c_L, \rho^s_L)^T$, where $\rho^c_L$ and $\rho^s_L$ are the derivatives of $Z_L(k)$ and $Z_L(v)$, respectively. After taking the thermodynamic limit, we can derive a set of functional equations for the densities of the rapidities (see Appendix B)

$$\rho_L(k,v) = \rho^0(k,v) + \frac{1}{L} \tau^0(k,v) + \frac{\sigma^0_1(k,v)}{24L^2 \rho^+_L(k^+)} + \frac{\sigma^0_2(k,v)}{24L^2 \rho^+_L(v^+)}$$

$$+ K(k,v,|k',v'|) \rho_L(k',v')$$

$$(3.3)$$

where $K$ is the matrix operator (B.12) and $\rho^0, \tau^0, \sigma^0_1$ and $\sigma^0_2$ are the densities defined in (B.14). The solution of the equation (3.3) is given by

$$\rho_L(k,v) = \rho(k,v) + \frac{1}{L} \tau(k,v) + \frac{\sigma_1(k,v)}{24L^2 \rho^+_L(k^+)} + \frac{\sigma_2(k,v)}{24L^2 \rho^+_L(v^+)}.$$  

$$(3.4)$$

We introduce the following notation

$$(a, b) \equiv \int_{-k^+}^{k^+} a(k)b(k)dk + \int_{-v^+}^{v^+} a^*(v)b^*(v)dv$$

$$(3.5)$$
Then the energy density \( e_L \) of the finite system is given by

\[
e_L(k^+, v^+) = \frac{E}{L} = (e^0, \rho_L)
\]

where

\[
e^0 = (\mu_s - \cos k, h_s)^T
\]

\[
\mu_s = \mu/2 - h/4, \quad h_s = h/2.
\]

From the solution (3.4) we have

\[
e_L(k^+, v^+) = e_\infty(k^+, v^+) + \frac{1}{L} e_{\text{sur}}(k^+, v^+) - \frac{1}{24L^2}(\epsilon_1(k^+, v^+) + \epsilon_2(k^+, v^+))
\]

where the bulk energy density \( e_\infty \) of the infinite system, the surface energy \( e_{\text{sur}}, \epsilon_1 \) and \( \epsilon_2 \) are given by

\[
e_\infty(k^+, v^+) = (e^0, \rho), \quad e_{\text{sur}}(k^+, v^+) = [1 - \mu_s - h_s + (e^0, \sigma)],
\]

\[
\epsilon_1(k^+, v^+) = \frac{1}{\rho_L^0(k^+)}[2 \sin k^+ - (e^0, \sigma_1)],
\]

\[
\epsilon_2(k^+, v^+) = -\frac{1}{\rho_L^0(v^+)}(e^0, \sigma_2).
\]

Let us consider the ground state of the infinite system. We denote by \( k^0 \) and \( v^0 \) the Fermi surfaces of the charge and spin rapidities, respectively. (See also Appendix B.) Let us denote by \( n^c \) and \( n^s \) the number density of all electrons and that of down-spin electrons, respectively: \( n^c = N/L \) and \( n^s = M/L \). In the ground state of the infinite system they are related to the Fermi surfaces by

\[
n^c_0 = \lim_{L \to \infty} \frac{N}{L} = \frac{1}{2} \int_{-k^0}^{k^0} \rho^c(k) dk, \quad n^s_0 = \lim_{L \to \infty} \frac{M}{L} = \frac{1}{2} \int_{-v^0}^{v^0} \rho^s(v) dv
\]

Then, the changes of the variables \( N \) and \( M \) from the ground state are defined by

\[
\Delta N = N - Ln^c_0, \quad \Delta M = M - Ln^s_0.
\]

We note that \( \Delta N \) and \( \Delta M \) also depend on certain commensurate conditions for \( N, M \) and \( L \), as discussed in Ref. [3]. Thus, for the low-excited states due to the shift of \( N \) or \( M \), the finite-size correction is given by

\[
e_L(N, M) = e_\infty(k^0, v^0) + \frac{1}{L} e_{\text{sur}}(k^0, v^0)
\]
\[ + \frac{\varepsilon_1}{L^2} \left\{ \left[ (\Delta N + 1/2 - B_c)\xi_{22} - (\Delta M + 1/2 - B_s)\xi_{21} \right]^2 - \frac{1}{24} \right\} \]
\[ + \frac{\varepsilon_2}{L^2} \left\{ \left[ (\Delta M + 1/2 - B_s)\xi_{11} - (\Delta N + 1/2 - B_c)\xi_{12} \right]^2 - \frac{1}{24} \right\} \]

where

\[ B_c = \frac{1}{2} \int_{-k^0}^{k^0} \tau^c(k)dk \]
\[ B_s = \frac{1}{2} \int_{-v^0}^{v^0} \tau^s(v)dv. \] (3.12)

Here we have used the dressed charge matrix \( \xi = \xi(k = k^0, v = v^0) \) defined by

\[ \xi(k, v) = 1 + K^T(k, v|k', v')\xi(k', v'), \] (3.13)

where the matrix operator \( K^T \) is given in (B.13) in Appendix B.

We now consider the particle-hole excitation. The particle and hole excitations near the Fermi surfaces can be characterized by the quantum numbers \( I_p \) and \( I_h \) for the charge sector, and \( J_p \) and \( J_h \) for the spin sector.

\[ Z^c_L(k_p) = \frac{I_p}{L}, \quad Z^c_L(k_h) = \frac{I_h}{L} \]
\[ Z^s_L(v_p) = \frac{J_p}{L}, \quad Z^s_L(v_h) = \frac{J_h}{L} \] (3.14)

The presence of these kinds of excitations modifies \( \rho_L \) by \(-\sigma_1(k, v)(k_p - k_h)/L \) and \(-\sigma_2(k, v)(v_p - v_h)/L \). The energy contributions of the particle-hole pairs of the spin and charge sectors are given by \( \varepsilon_1(k^+, v^+)(I_p - I_h)/L \) and \( \varepsilon_2(k^+, v^+)(J_p - J_h)/L \), respectively. The “momenta” of the excitations are considered as \( \pi(I_p - I_h)/L \) and \( \pi(J_p - J_h)/L \), respectively. Therefore, the Fermi velocities are defined by \( \varepsilon_F^c = \varepsilon_1(k^0, v^0)/\pi \) and \( \varepsilon_F^s = \varepsilon_2(k^0, v^0)/\pi \). Thus, we obtain the complete form of the finite-size correction of the energy

\[ e_L(N, M) = e_{\infty}(k^0, v^0) + \frac{1}{L} \left[ 1 - \mu_s - h_s + (e^0, \tau) \right] \]
\[ + \frac{\pi \varepsilon_F^c}{L^2} \left\{ \left[ (\Delta N + 1/2 - B_c)\xi_{22} - (\Delta M + 1/2 - B_s)\xi_{21} \right]^2 - \frac{1}{24} + N_{ph}^c \right\} \]
\[ + \frac{\pi \varepsilon_F^s}{L^2} \left\{ \left[ (\Delta M + 1/2 - B_s)\xi_{11} - (\Delta N + 1/2 - B_c)\xi_{12} \right]^2 - \frac{1}{24} + N_{ph}^s \right\} \] (3.15)
where

\[ N_{ph}^c = \sum_j I_{p_j} - I_{h_j} \quad N_{ph}^s = \sum_m J_{p_m} - J_{h_m}. \]

Let us compare the energy spectrum (3.15) of the open-boundary case with that of the periodic case. We consider the energy of the 1D Hubbard Hamiltonian under the periodic boundary condition with \( L \) sites, where \( N_c \) and \( N_s \) are the number of total electrons and that of down spins, respectively. The finite-size correction of the periodic case, the eq. (2.44) in Ref. [3], is given in the following.

\[
E_{\text{periodic}} = L e_{\text{periodic}}^\infty + 2\pi v_c L \left\{ \frac{[\xi_{22}(N_c - \nu_c L) - \xi_{21}(N_s - \nu_s L)]^2}{4(\det\xi)^2} + (\xi_{11} D_c + \xi_{12} D_s)^2 - \frac{1}{12} + N_{ph}^c \right\} \\
+ 2\pi v_s L \left\{ \frac{[\xi_{12}(N_c - \nu_c L) - \xi_{11}(N_s - \nu_s L)]^2}{4(\det\xi)^2} + (\xi_{21} D_c + \xi_{22} D_s)^2 - \frac{1}{12} + N_{ph}^s \right\}.
\]

(3.16)

Here \( 2D_c \) and \( 2D_s \) are the momenta of state in units of the Fermi momenta, and \( \nu_c \) and \( \nu_s \) are the number densities of total electrons and down-spin electrons, respectively, which are defined for the infinite system. They satisfy the selection rules

\[
D_c = (\Delta N_c + \Delta N_s)/2 \quad (\mod 1), \quad D_s = \Delta N_c/2 \quad (\mod 1). \quad (3.17)
\]

From the comparison of the open boundary case with the periodic one, we observe the following properties of the energy spectrum under the open-boundary conditions: (i) there is no particle moving from the left Fermi surface to the right one (no \( D_c \) or \( D_s \) for the open case); (ii) there are no selection rules; (iii) the factors \( 1/2 - B_c \) and \( 1/2 - B_s \) give nontrivial contributions due to the boundary conditions.

In the open-boundary case (3.15), the terms \( 1/2 - B_c \) and \( 1/2 - B_s \) are not integer-values, in general. \( B_c \) and \( B_s \) can change continuously with respect to the boundary fields \( p_{1\uparrow} \) and \( p_{L\uparrow} \) together with the Fermi surfaces \( k^0 \) and \( v^0 \) through the relations (3.12) and the integral equations. Thus, the \( O(1/L^2) \)-corrections of the spectrum of the open-boundary Hubbard model under the boundary fields are quite different from those of the periodic-boundary condition. We shall discuss some physical interpretations of the spectrum and the conformal dimensions for several interesting cases in §4 and §5.

4 BCFT interpretations for the band less than half-filling

We shall discuss several physical implications of the energy spectrum of the open-boundary Hubbard model from the viewpoint of the boundary conformal field theories
(BCFT). We consider the case of the band which is less than half-filling in §4, and the case at the half-filling in §5.

4.1 BCFT spectrum with the phase shift

Let us consider the spectrum (3.15) of the open-boundary Hubbard model from the viewpoint of BCFT. The finite-size correction (3.15) can be expressed as follows

$$E = L e_\infty + e_{\text{sur}} + \frac{\pi v_c^c}{L} \left(-\frac{1}{24} + \Delta_c\right) + \frac{\pi v_s^s}{L} \left(-\frac{1}{24} + \Delta_s\right) + o\left(\frac{1}{L}\right)$$

(4.1)

where $\Delta_c$ and $\Delta_s$ are given by

$$\Delta_c = \frac{1}{2} \left(\frac{(\Delta N + 1/2 - B_c)\xi_{22} - (\Delta M + 1/2 - B_s)\xi_{21}}{2 \det \xi}\right)^2 + N_{\text{ph}}^c$$

$$\Delta_s = \frac{1}{2} \left(\frac{(\Delta M + 1/2 - B_s)\xi_{11} - (\Delta N + 1/2 - B_c)\xi_{12}}{2 \det \xi}\right)^2 + N_{\text{ph}}^s$$

(4.2)

We see that the $O(1/L)$-terms of the spectrum of the open-boundary Hubbard model are very similar to the sum of the conformal dimensions of two chiral conformal field theories with $c = 1$. The fact that the spectrum (4.1) is expressed only with the chiral components is consistent with the standard finite-size spectrum [1] of the boundary conformal field theories.

The BCFT viewpoint also makes clear the difference between the open-boundary spectrum (3.15) and the periodic one. In Refs. [14, 15] the finite-size spectrum of Hubbard model under the periodic-boundary condition is discussed from the CFTs with $c = 1$, and it is expressed in terms of the sum of the chiral and antichiral components of the conformal dimensions.

$$E_{\text{periodic}} = L e_\infty + e_{\text{periodic}} + \frac{2\pi v_c^c}{L} \left(-\frac{1}{12} + \Delta_c + \bar{\Delta}_c\right) + \frac{2\pi v_s^s}{L} \left(-\frac{1}{12} + \Delta_s + \bar{\Delta}_s\right) + o\left(\frac{1}{L}\right),$$

(4.3)

where the symbols $\Delta$ and $\bar{\Delta}$ denote the chiral and antichiral components of the conformal dimensions, respectively.

Let us consider the terms $B_c$ and $B_s$ in (3.15) or (4.2). We may regard them as a certain ‘phase shifts’. [7] For an illustration, we calculate the spectrum of a bosonic open-string with length $\pi$ under the Dirichlet boundary condition. [23] Let us introduce the action $S$ by

$$S = \int_{-\infty}^{\infty} dt \int_0^\pi d\sigma \frac{1}{2\pi} \left\{ \left(\frac{\partial \varphi}{\partial t}\right)^2 - \left(\frac{\partial \varphi}{\partial \sigma}\right)^2 \right\}$$

(4.4)
From the canonical quantization we have
\[
\varphi(\sigma, t) = w\sigma + \sum_{m \neq 0} \frac{1}{n} \alpha_m \sin m\sigma e^{-int} \tag{4.5}
\]
where the boson operators \(\{\alpha_m\}\) have the commutation relations \([\alpha_m, \alpha_n] = m\delta_{m+n,0}\).

Let us consider the “compactification” of the open string with radius \(R\). Since the string is fixed at the boundaries, it may have a phase shift \(\delta\):
\[
\varphi(\pi, t) = \varphi(0, t) + 2\delta R \pmod{2\pi R} \tag{4.6}
\]
Therefore the zero-mode \(w\) is given by
\[
w = 2R \left( \hat{N} + \frac{\delta}{\pi} \right) \tag{4.7}
\]
where \(\hat{N}\) is an integer. We note that the variable \(\delta\) can also be considered as the phase shift due to the scattering at a boundary. The Hamiltonian of the open string is given by
\[
\hat{H} = \frac{1}{2\pi} \int_0^\pi \left\{ \left( \frac{\partial \varphi}{\partial t} \right)^2 + \left( \frac{\partial \varphi}{\partial \sigma} \right)^2 \right\} \\
= \frac{w^2}{2} + \frac{1}{2} \sum_{m \neq 0} \alpha_m \alpha_{-m} \\
= \frac{1}{2}(2R)^2 \left( \hat{N} + \frac{\delta}{\pi} \right)^2 + \sum_{m=1}^\infty \alpha_{-m} \alpha_m - \frac{1}{24} \tag{4.8}
\]
Thus, the spectrum of the bosonic open-string under the Dirichlet boundary condition is described by the chiral CFT with \(c = 1\) and the phase shift \(\delta\). The conformal dimension \(\Delta\) is given by
\[
\Delta = \frac{1}{2}(2R)^2 \left( \hat{N} + \frac{\delta}{\pi} \right)^2 + \sum_{m=1}^\infty mn_m \tag{4.9}
\]
where \(n_m\) is the excitation number of the mode \(\alpha_m\).

We consider that the spectrum (4.1) of the open-boundary Hubbard model can be described by the two chiral conformal field theories of \(c = 1\) with boundaries. Applying the spectrum (4.8) and the conformal dimension (4.9) of the open string to the finite-size correction (3.15) and (4.2) we shall derive a number of physical interpretations, in later sections.
We now introduce some symbols so that we express the four different open-boundary conditions explicitly.

\[ \alpha_1 \text{ denotes that } p_{1\uparrow} = +p_{1\downarrow} \text{ or } p_{1\uparrow} = -p_{1\downarrow} = \pm \infty, \]
\[ \beta_1 \text{ denotes that } p_{1\uparrow} = -p_{1\downarrow} \neq 0, \pm \infty, \]
\[ \alpha_L \text{ denotes that } p_{L\uparrow} = +p_{L\downarrow} \text{ or } p_{L\uparrow} = -p_{L\downarrow} = \pm \infty, \]
\[ \beta_L \text{ denotes that } p_{L\uparrow} = -p_{L\downarrow} \neq 0, \pm \infty. \] (4.10)

The four cases of the open-boundary conditions are expressed as \( \alpha_1 \alpha_L, \beta_1 \alpha_L, \alpha_1 \beta_L, \) and \( \beta_1 \beta_L. \) We also define the following symbols

\[ b_1 = \frac{U}{4} + \frac{(p_{1\uparrow} - p_{1\downarrow}^{-1})}{2}, \quad \bar{b}_L = \frac{U}{4} + \frac{(p_{L\uparrow} - p_{L\downarrow}^{-1})}{2} \] (4.11)

We introduce the step function \( s(x) \) in the following: \( s(x) = 1 \) for \( x > 0, \) and \( s(x) = -1 \) for \( x < 0. \)

### 4.2 Conformal dimensions under zero magnetic field: \( h = 0 \)

Let us consider the integral equations for the dressed charge. Under zero magnetic field, there is no magnetization in the ground state of the infinite system. The parameter \( v^0 \) is given by \( \infty, \) and the set of the integral equations reduces to scalar ones by using the Fourier transformation. Through the Wiener-Hopf method the dressed charge matrix is given by

\[
\xi = \begin{pmatrix} \xi_{11} & \xi_{12} \\ \xi_{21} & \xi_{22} \end{pmatrix} = \begin{pmatrix} \xi(k^0) & \xi(k^0)/2 \\ 0 & 1/\sqrt{2} \end{pmatrix}
\] (4.12)

where

\[
\xi(k) = 1 + \frac{1}{2} \int_{-k^0}^{k^0} \xi(k') \tilde{K} \sin(k) \sin(k') \cos(k') dk',
\]
\[
\tilde{K}(x) = \frac{1}{2} \int_{-\infty}^{\infty} e^{i\omega x} \frac{e^{i\omega U/2}}{1 + e^{i\omega U/2}} d\omega.
\] (4.13)

Thus, the conformal dimensions (4.2) of the spectrum (4.1) of the open-boundary Hubbard model are written in the following

\[
\Delta_c = \frac{1}{2\xi^2} (\Delta N + 1/2 - B_c)^2 + N_{ph}^c \] (4.14)
\[
\Delta_s = \frac{1}{4} (2\Delta M - \Delta N + (1/2 + B_c - 2B_s))^2 + N_{ph}^s \] (4.15)
where
\[
\frac{1}{2} - B_c = \frac{1}{2} - \frac{1}{2} \int_{-k_0}^{k_0} \tau^c(v) dv
\]  
(4.16)
and
\[
\frac{1}{2} + B_c - 2B_s = \frac{1}{2} \times \begin{cases} 
0 & \alpha_1 \alpha_L \\
\beta_1 \alpha_L & s(b_1) \\
\alpha_1 \beta_L & s(b_L) \\
\beta_1 \beta_L & s(b_1) + s(b_L)
\end{cases}
\]  
(4.17)

Here we recall that \(s(x)\) denotes the step function, and also that \(b_j = U/4 - (p^{-1}_j - p_{j1})/2\) for \(j = 1\) and \(L\).

Let us define \(R_c, R_s, \delta_c\) and \(\delta_s\) by the following
\[
2R_c = \frac{1}{\xi}, \quad \delta_c = \pi \left( \frac{1}{2} - B_c \right),
\]  
(4.18)
\[
2R_s = \frac{1}{\sqrt{2}}, \quad \delta_s = \pi \left( \frac{1}{2} + B_c - 2B_s \right).
\]  
(4.19)

Then the expressions of the dimensions (4.14) and (4.15) are consistent with that of the conformal dimensions (4.3). Thus we conclude that the charge and spin excitations of the open-boundary Hubbard model under zero magnetic field can be described by the boundary CFTs with \(c = 1\), where the radii \(R_c, R_s\) and the phase shifts \(\delta_c, \delta_s\) are given by (4.18) and (4.19). Here we observe the following facts: (i) the parameter \(\xi\) can be changed continuously with respect to the filling factor \(n_0\); (ii) the value of the dimension \(\Delta_s\) is given by an integer multiplied by 1/4 (\(\Delta_s \in \mathbb{Z}/4\)). The latter reminds us the conformal dimensions of the affine SU(2) with level 1. We may consider that the facts (i) and (ii) reflect \(U(1)\) and \(SU(2)\) symmetries, respectively.

In [20] the spectrum of the open-boundary Hubbard model is discussed from the viewpoint of the shifted \(U(1)\) Kac-Moody algebra [24] for the special case of the boundary condition \(\alpha_1 \alpha_L\). In the shifted \(U(1)\) Kac-Moody algebra, the spectrum also has an “shift”. Thus the CFT interpretation in [20, 24] is different from that of the present paper.

### 4.3 \(\pi/2\)-phase shift due to magnetic impurity at the boundaries

We discuss the conformal dimensions \(\Delta_s\) of the spin excitations under zero magnetic field from the viewpoint of the impurity scattering with \(\pi/2\)-phase shift. In Table 1 the values of the zero-mode part of \(\Delta_s\) (4.15) are shown for the \(3 \times 3\) different boundary conditions.
Here we recall

\[ b_1 = U/4 + (p_{1\uparrow} - p_{1\uparrow}^{-1})/2, \quad b_L = U/4 + (p_{L\uparrow} - p_{L\uparrow}^{-1})/2. \]

From Table 1 we see that the conformal dimension \( \Delta_s \) is quite sensitive to the change of the boundary magnetic fields \( p_{1\uparrow} \) and \( p_{L\uparrow} \); it takes quantized values of some integral multiple of 1/4 \( (\Delta_s \in \mathbb{Z}/4) \) and it takes different values under the different boundary conditions. For an illustration we consider the case when the boundary chemical potentials are given by zero or infinitesimally small. This corresponds to the boundary condition denoted by \( \alpha_1 \alpha_L \) where there is no phase shift: \( \delta_s = 0 \). If we add a very small boundary magnetic field \( p_{1\uparrow} \) at the site 1 and keep the boundary chemical potential at the site \( L \) unchanged, the new boundary condition corresponds to the case of \( \beta_1 \alpha_L \) with \( b_1 < 0 \). Then the phase shift \( \delta_s \) becomes \( \pi/2 \), which is distinct from 0. Furthermore, the change is quantized.

The \( \pi/2 \)-phase shift of the spin excitation is quite similar to that of the electron scattering at a certain magnetic impurity such as in the Kondo problem, where the \( \pi/2 \)-phase shift corresponds to the unitarity limit of the scattering. \[26\] We may consider that under the boundary magnetic fields, the boundary sites 1 and \( L \) play the role of the magnetic impurity for the open-boundary Hubbard model.

From the viewpoint of the scattering at the magnetic impurity we can explain the result in Table I. For the case of \( \alpha_1 \alpha_L \) there is no boundary magnetic fields and the phase-shift \( \delta_s \) of the spin sector is given by 0. For the cases of \( \alpha_1 \beta_L \) or \( \beta_1 \alpha_L \), there is an magnetic impurity at one of the sites 1 or \( L \) and the phase-shift is given by \( \pm \pi/2 \). For the cases of \( \beta_1 (b_1 > 0) \beta_L (b_L < 0) \) and \( \beta_1 (b_1 < 0) \beta_L (b_L > 0) \), the phase-shifts from the two impurities at the boundaries have different signs and they cancel each other out. Thus the total phase shift is given by 0. For the cases of \( \beta_1 (b_1 > 0) \beta_L (b_L > 0) \)

| \( \Delta_s \) | \( \alpha_1 \) | \( \beta_1 \) |
| --- | --- | --- |
| \( \alpha_L \) | \( \frac{1}{4}(2\Delta M - \Delta N)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N - 1/2)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N + 1/2)^2 \) |
| \( \beta_L \) | \( \frac{1}{4}(2\Delta M - \Delta N - 1/2)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N - 1)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N)^2 \) |
| \( b_L > 0 \) | \( \frac{1}{4}(2\Delta M - \Delta N + 1/2)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N + 1)^2 \) |
| \( b_L < 0 \) | \( \frac{1}{4}(2\Delta M - \Delta N + 1/2)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N)^2 \) | \( \frac{1}{4}(2\Delta M - \Delta N + 1)^2 \) |

Table I
and $\beta_1(b_1 < 0)\beta_L(b_L < 0)$, the phase-shifts from the two boundary magnetic impurities have the same sign and the total phase shift is given by $\pm \pi$.

The phase shift $\delta_s$ depends on the Coulomb interaction among the band electrons for the finite-size spectrum of the open-boundary Hubbard model. The parameter $b_1$ ($b_L$) depends on both the Coulomb coupling constant $U$ and the boundary magnetic field $p_{1\uparrow}$ ($p_{L\uparrow}$), and the sign of $b_1$ ($b_L$) can be changed by controlling $U$. For the Kondo problem, the $\pi/2$ phase-shift is related to the boundary operator with the scaling dimension $1/4$. \cite{27, 5, 7} However, the phase shift does not depend on the Coulomb interaction among electrons.

There are some models for the impurity scattering of electrons. We first note that for the Kondo model there is no Coulomb interaction among the electrons. For the Anderson model, the electrons have the Coulomb repulsion only on the impurity site; there is no Coulomb interaction among the band electrons of the Anderson model, whose wave functions are given by plane waves. For the Wolff model, the band electrons interact through the Coulomb repulsion not only on the impurity site but also on each site of the lattice such as in the Hubbard model. \cite{28, 29, 30} Thus we consider that the impurity effect of the open-boundary Hubbard model may have some properties in common with that of the Wolff model. Unfortunately, however, no exact solution is known for the Wolff model. It will be an interesting problem if we can discuss the magnetic properties of the Wolff model from some exact results of the 1D Hubbard model under the open boundary conditions.

### 4.4 Fermi-edge singularity due to the boundary impurity

We discuss the spectrum \cite{12} of the open-boundary Hubbard model from the viewpoint of the Fermi-edge singularity of the X-ray spectrum. \cite{12} For simplicity, we consider the case of zero magnetic field. We assume that the boundary sites play the role of the impurity atoms. Let us introduce the following operator

$$H_B = \sum_\sigma p_{1\sigma} c_{1\sigma}^\dagger b_{1\sigma} b_{1\sigma}^\dagger + \sum_\sigma p_{L\sigma} c_{L\sigma}^\dagger c_{L\sigma} b_{L\sigma} b_{L\sigma}^\dagger. \quad (4.20)$$

Here the operators $b_1$ and $b_L$ annihilate the ionic deep core electrons of the boundary "atoms". \cite{4, 21} The operators can be considered as the creation operators of the holes at the boundary sites. The dimension of the operator $b$ (and $b^\dagger$) is closely related to the singularity in the X-ray absorption probability. \cite{1, 21} We denote by $\mathcal{H}'$ the Hamiltonian which is derived from the open-boundary Hubbard Hamiltonian \cite{12} by
replacing the boundary terms with $H_B$

$$\mathcal{H} = -\sum_{j=1}^{L-1} \sum_{\sigma=\uparrow, \downarrow} (c_{j\sigma}^\dagger c_{j+1\sigma} + c_{j+1\sigma}^\dagger c_{j\sigma}) + U \sum_{j=1}^{L} n_{j\uparrow} n_{j\downarrow} + \mu \sum_{j=1}^{L} (n_{j\uparrow} + n_{j\downarrow})$$

$$- \frac{\hbar}{2} \sum_{j=1}^{L} (n_{j\uparrow} - n_{j\downarrow}) + H_B \quad (4.21)$$

The spectrum of (4.21) can be derived from that of the open-boundary Hubbard model (1.2).

Let us discuss the one-impurity effect of the boundary chemical potential. We consider the case when $p_{1\sigma} = p$ and $p_{L\sigma} = 0$ for $\sigma = \uparrow, \downarrow$, or the case when $p_{1\sigma} = 0$ and $p_{L\sigma} = p$ for $\sigma = \uparrow, \downarrow$. Furthermore, we assume that the boundary chemical potential is very small. Then from the integral equation of $\tau$, for small boundary chemical potential ($|p| \to 0$), we find

$$B_p^c = B_c^0 + \sum_{n=1}^{\infty} (-1)^n p^na_n,$$

$$B_c^0 = \frac{1}{2} \int_{-k^0}^{k^0} a(k) dk,$$

$$a_n = \frac{1}{2} \int_{-k^0}^{k^0} a_n(k) dk, \quad n \geq 1,$$

where

$$a_n(k) = \frac{\cos(nk)}{\pi} + \frac{\cos k}{2\pi} \int_{-k^0}^{k^0} \tilde{K}(\sin k - \sin k') a_n(k') dk'$$

$$a(k) = \frac{1}{2\pi} \left(2 - \frac{U/2 \cos k}{\sin^2 k + (U/4)^2}\right) + \frac{\cos k}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i\omega/2}}{2 \cosh(\omega U/4)} e^{-i\omega \sin k} d\omega$$

(4.23)

Here, the superscript $p$ (0) stands for the system with (without) a boundary hole. It is easy to show $0 < B_c^p < 1$ and $0 < B_c^0 < 1$. Thus, the energy spectra for two systems are

$$E^0 = L e_\infty + f_\infty(0) + \frac{\pi}{L} \left\{ \frac{v_c}{\xi^2} [(\Delta N + 1/2 - B_c^0)^2 - \frac{1}{24}] + v_s[(\Delta M - \Delta N/2)^2 - \frac{1}{24}] \right\}$$

$$E^p = L e_\infty + f_\infty(p) + \frac{\pi}{L} \left\{ \frac{v_c}{\xi^2} [(\Delta N + 1/2 - B_c^p)^2 - \frac{1}{24}] + v_s[(\Delta M - \Delta N/2)^2 - \frac{1}{24}] \right\}$$

(4.24)
Let us regard the operator $b$ as the boundary changing operator. If we could define the scaling dimension of $b$ for $|p| \sim 0$ (up to $p^2$), then it would be given by

$$x_b = \frac{1}{\xi^2} \left( \frac{\delta_c^p}{\pi} \right)^2 - \frac{1}{\xi^2} \left( \frac{\delta_c^0}{\pi} \right)^2 = \frac{L}{\pi v_c} (E_g^p - E_g^0 - f_\infty(p) + f_\infty(0))$$

$$= \left\{ p(1 - 2B^0_c)a_1 + p^2[(a_1)^2 + (1 - 2B^0_c)a_2] \right\} /\xi^2$$

(4.25)

where the subscript $g$ stands for the ground state ($\Delta N = \Delta M = 0$). We recall that $\delta_c^p$ and $\delta_c^0$ denote the phase shifts for the case $p \neq 0$ and $p = 0$, respectively. If $2B^0_c = 1$, then we have $\delta_c^0 = 0$. We may consider that the contribution of $\delta_c^0$ to $x_b$ is due to the electron interaction.

Let us introduce the creation operator $\psi^\dagger$ for down-spin electrons, which increases the number $N$ of total electrons by 1 and that of down electrons $M$ by 1. The operator $b\psi^\dagger$ maps the ground state with no boundary hole into the state with a boundary hole and $N_0 + 1$ electrons present. Let us consider the energy difference

$$E_1^p - E_g^0 - (f_\infty(p) - f_\infty(0)) = \frac{\pi v_c}{L\xi^2} \{(3/2 - B^p_c)^2 - (1/2 - B^0_c)^2\} + \frac{\pi v_s}{4L}$$

(4.26)

We note that $v_c \neq v_s$, in general. The energy difference (4.26) is related to both the charge and spin excitations. Let us assume that the operator $b\psi^\dagger$ is a composite operator of $(b\psi^\dagger)_c$ in charge sector and $(b\psi^\dagger)_s$ in spin sector. The scaling dimensions are given by

$$x_{(b\psi)_c} = (1 - 2B^0_c)(1 + pa_1 + p^2a_2) /\xi^2 + (1 + pa_1 + p^2a_2)^2 /\xi^2$$

(4.27)

$$x_{(b\psi)_s} = \frac{1}{4}$$

The term proportional to $(1 - 2B^0_c)$ in the dimension (4.27) can be considered as the effect of the Coulomb interaction among the electrons.

### 4.5 Exact solutions of a two-impurity problem

In the last two subsections, we have discussed the effects of the impurities at the site 1 and $L$, separately and independently. However, we can discuss the correlation between the two impurities at the sites 1 and $L$ by investigating how the energy spectrum changes under the different open-boundary conditions.

For an illustration, we consider the dimension $\Delta_s$ of the spin excitation under zero magnetic field (see Table 1). Let us denote by $\delta_{s1}$ and $\delta_{sL}$ the phase shifts due to the boundaries 1 and $L$, respectively. We recall that under zero magnetic field the total phase shift $\delta_s$ can be consider as the sum $\delta_s = \delta_{s1} + \delta_{sL}$. Here we assume that for the charge excitations $\Delta N = 0$ gives the lowest value of the dimension $\Delta_c$. Then, for the
case of \( \beta_1(b_1 > 0)\beta_L(b_L > 0) \), the value of \( \Delta_s \) is degenerate for \( \Delta M = 0 \) and 1. For the case of \( \beta_1(b_1 < 0)\beta_L(b_L < 0) \), it is degenerate for \( \Delta M = 0 \) and -1. Thus the finite-size spectrum can be changed under the different open-boundary conditions with respect to the boundary magnetic fields. We may regard the change as the interaction between the two impurities.

The spin and charge excitations of the spectrum (4.1) are coupled to each other, in general. In order to make a quantitative analysis on the change of the spectrum under the different open-boundary conditions, we should evaluate the coupled integral equation of \( \tau \).

\[
\tau(k, v) = \tau^0(k, v) + K(k, v|k', v')\tau(k', v')
\]

The integral equation describes the effect of the electron interaction on the impurities; the impurity should be dressed with the Coulomb interaction among electrons. Here we recall that \( \tau^0 \) is given by the sum of the contributions of the two impurities and the ‘zero mode’ (see (3.2) and (3.3)). Thus we can decompose \( \tau \) into three parts: \( \tau_1 \), \( \tau_L \) and \( \tau_{\text{zero}} \) which are contributions from the sites 1 and \( L \), and the ‘zero mode’. Unfortunately, however, it is not so easy to solve the integral equation analytically.

For the Kondo problem, the effect of two magnetic impurities gives a quite nontrivial problem. \([32, 33]\) It will be an interesting future problem to discuss the effect of the different boundary conditions in the spectrum of the open-boundary Hubbard model from the viewpoint of the Kondo problem. Through some numerical evaluation of \( \tau \) for general values of the magnetic field \( h \) and the chemical potential \( \mu \), we can investigate some aspects of the two impurity effect, exactly. This problem should be discussed elsewhere.

### 4.6 Under a strong magnetic field: \( h > h_c \)

If the magnetic field \( h \) is large enough \( h \geq h_c \), then the ground state of the Hubbard model is given by a ferromagnetic state corresponding to \( v^0 = 0 \), and all the electrons are spin-up. Here \( h_c \) denotes the critical value of the magnetic field. \([14]\) The dressed charge matrix is given by \( \xi_{11} = \xi_{22} = 1, \xi_{12} = 0, \xi_{21} = (2/\pi)\tan^{-1}(\sin(4\pi n_c)/U) \). The critical magnetic field is evaluated as

\[
h_c = \frac{U}{2\pi} \int_{-\pi n_c}^{\pi n_c} dk \cos(k) \frac{\cos(k) - \cos(\pi n_c)}{(U/4)^2 + \sin^2(k)}
\]

The conformal dimensions are given by

\[
\Delta_c = \frac{1}{2}(\Delta N + 1/2) - \frac{1}{\pi} \left\{ \tan^{-1}\left( \frac{p_{11}^1 + \cos(\pi n_c)}{\sin(\pi n_c)} \right) + \tan^{-1}\left( \frac{p_{11} + \cos(\pi n_c)}{\sin(\pi n_c)} \right) \right\}^2
\]

\[
\Delta_s = \frac{1}{2}(\Delta M + 1/2)^2.
\]
The conformal dimension for the charge sector depends on the boundary magnetic fields, while that of the spin sector is independent of the boundary fields.

5 Conformal dimensions at the half-filling

For the half-filling case, the parameter \( k^0 = \pi \). Thus we can only consider the spin sector in the set of integral equations. The elements of the dressed charge matrix are given by \( \xi_{11} = 1, \xi_{21} = 0 \) and

\[
\xi_{22}(v) = 1 - \frac{1}{2\pi} \int_{-\phi}^{\phi} dv \xi_{22}(v') K_2(v - v'),
\]

\[
\xi_{12}(k) = \frac{1}{2\pi} \int_{-\phi}^{\phi} dv \xi_{22}(v) K_1(\sin(k) - v).
\] (4.30)

Since the parameter \( \phi \) depends on the magnetic field \( h \), we discuss the three cases: 

5.1 \( a: \quad h \geq h_c \)

Since \( k^0 = \pi \), the integral of \( \tau^c(k) \) over \( -\pi \) to \( \pi \) is zero. The constraint \( \phi = 0 \) leads to \( \xi_{22} = 1, \xi_{12} = 0 \). So, the ground state is ferromagnetic, and we have the following

\[
\Delta_s = \frac{1}{2}(\Delta M + 1/2)^2.
\] (4.31)

5.2 \( b: \quad h_c - h \sim 0 \)

The integral equation satisfied by \( \epsilon^s \) is

\[
\epsilon^s(v) = \frac{h}{2} - \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \cos^2(k) K_1(v - \sin(k)) - \frac{1}{2\pi} \int_{-\phi}^{\phi} dv' K_2(v - v') \epsilon^s(v')
\] (4.32)

From the condition \( \epsilon^s(\phi) = 0 \), we can get the following relation

\[
\phi = ((U/4)^2 + 1)^{3/4} h_c - h
\] (4.33)

and

\[
\xi_{22} = 1 - \frac{4((U/4)^2 + 1)^{3/4}}{U\pi} \sqrt{h_c - h}, \quad \xi_{12} = \frac{8((U/4)^2 + 1)^{3/4}}{U\pi} \sqrt{h_c - h}.
\] (4.34)
The conformal dimension is given by

$$\Delta_s = \frac{1}{2} \left( \frac{\Delta M + 1/2 - 4A_0/(U\pi)}{1 - 4v^0/(U\pi)} \right)^2 \frac{1}{2} \left( \frac{1/2 - 4A_0/(U\pi)}{1 - 4v^0/(U\pi)} \right)^2$$

(4.35)

where

$$A = \frac{2U}{4} \frac{U/4 + i\zeta_+}{U/4 + i\zeta_-} + 2 + \frac{U}{4} \int_{-\pi}^{\pi} K_1(\sin(k)) \tau^c_0(k) dk$$

The number of spin-down electrons at the ground state is given by

$$M = \left( \frac{L}{\pi} \right) \left( (U/4)^2 + 1 \right)^{1/4} \sqrt{h_c - h}$$

(4.36)

5.3 $c: \ h \sim 0$

The integral equations can be solved by using the Wiener-Hopf method. The dressed charge matrix was given by Frahm and Korepin [14, 15]

$$\xi_{22} = \left( 1 + (4\ln(h_0/h))^{-1} \right)/\sqrt{2}, \xi_{12} = 1/2 - 2h/(\pi^2 h_c), \xi_{21} = 0, \xi_{11} = 1$$

(4.37)

where $v^0 = (U/(2\pi)) \ln(h_0/h)$ and $h_0 = \sqrt{\pi^3/2eh_c}$. Applying the Wiener-Hopf method to the integral equation of $\tau$, we find $B_c = 0$ and

$$4B_s = \begin{cases} 1 - 4G^-(-i\pi/2)(h/h_0)^{2/|b|} & \alpha_1\alpha_L \\ 1 - 4G^-(-i\pi/2)(h/h_0)^{2/|b|} + s(b_1)(1 - 4G^-(-i\pi U/(4|h_0|))(h/h_0)^{2/|b_1|}) & \beta_1\alpha_L \\ 1 - 4G^-(-i\pi/2)(h/h_0)^{2/|b|} + s(b_1)(1 - 4G^-(-i\pi U/(4|h_0|))(h/h_0)^{2/|b_1|}) & \alpha_1\beta_L \\ 1 - 4G^-(-i\pi/2)(h/h_0)^{2/|b|} + s(b_1)(1 - 4G^-(-i\pi U/(4|h_0|))(h/h_0)^{2/|b_1|}) & \beta_1\beta_L \\ + s(b_1)(1 - 4G^-(-i\pi U/(4|h_0|))(h/h_0)^{2/|b_1|}) & \beta_1\beta_{b_L} \end{cases}$$

(4.38)

where

$$G^-(x\pi) = \frac{1}{\Gamma(1/2 + ix)} \sqrt{2\pi(ix)^{ix}e^{-ix}}$$

(4.39)

Substituting them into the finite-size corrections, we obtain the following result.
For case $\alpha_1 \alpha_L$:

$$\delta = 2 \left( \frac{(h/h_0)^{2/U} \sqrt{\pi/e} - h/(\pi^2 h_c)}{1 + (4 \ln(h/h_0))^{-1}} \right)$$  \hspace{1cm} (4.40)

For case $\alpha_1 \beta_L$:

$$\delta = \begin{cases} 
2 \left( \frac{(h/h_0)^{2/U} \sqrt{\pi/e} + (h/h_0)^{2/b_L} G^{-(-i\pi U/4b_L)} \frac{-h}{\pi^2 h_c} + \frac{1}{4}}{1 + \frac{1}{4 \ln(h/h_0)}} \right), & b_L > 0 \\
2 \left( \frac{(h/h_0)^{2/U} \sqrt{\pi/e} - (h/h_0)^{-2/b_L} G^{(-i\pi U/4b_L)} \frac{-h}{\pi^2 h_c} - \frac{1}{4}}{1 + \frac{1}{4 \ln(h/h_0)}} \right), & b_L < 0 
\end{cases}$$  \hspace{1cm} (4.41)

For case $\beta_1 \alpha_L$:

$$\delta = \begin{cases} 
2 \left( \frac{(h/h_0)^{2/U} \sqrt{\pi/e} + (h/h_0)^{2/b_1} G^{-(-i\pi U/4b_1)} \frac{-h}{\pi^2 h_c} + \frac{1}{4}}{1 + \frac{1}{4 \ln(h/h_0)}} \right), & b_1 > 0 \\
2 \left( \frac{(h/h_0)^{2/U} \sqrt{\pi/e} - (h/h_0)^{-2/b_1} G^{(-i\pi U/4b_1)} \frac{-h}{\pi^2 h_c} - \frac{1}{4}}{1 + \frac{1}{4 \ln(h/h_0)}} \right), & b_1 < 0 
\end{cases}$$  \hspace{1cm} (4.42)
For case $\beta_1 \beta_L$, $\delta/\pi$ is equal to

\[
\begin{cases}
2 \left( \frac{h}{\hbar_0} \frac{2}{U} \sqrt{\frac{\pi}{e}} + \left( \frac{h}{\hbar_0} \right)^{2/b_1} G^{-\frac{i\pi U}{4b_1}} + \left( \frac{h}{\hbar_0} \right)^{2/b_L} G^{-\frac{i\pi U}{4b_L}} - \frac{h}{\pi^2 h_c} + \frac{1}{2} \right) \\
\frac{1}{4\ln(h/\hbar_0)} 
\end{cases}
\]

\[b_1 > 0, b_L > 0\]

\[
2 \left( \frac{h}{\hbar_0} \frac{2}{U} \sqrt{\frac{\pi}{e}} + \left( \frac{h}{\hbar_0} \right)^{2/b_1} G^{-\frac{i\pi U}{4b_1}} - \left( \frac{h}{\hbar_0} \right)^{-2/b_L} G^{-\frac{i\pi U}{4b_L}} - \frac{h}{\pi^2 h_c} \right) \\
\frac{1}{4\ln(h/\hbar_0)}
\]

\[b_1 > 0, b_L < 0\] (4.43)

\[
2 \left( \frac{h}{\hbar_0} \frac{2}{U} \sqrt{\frac{\pi}{e}} - \left( \frac{h}{\hbar_0} \right)^{-2/b_1} G^{-\frac{i\pi U}{4b_1}} + \left( \frac{h}{\hbar_0} \right)^{2/b_L} G^{-\frac{i\pi U}{4b_L}} - \frac{h}{\pi^2 h_c} \right) \\
\frac{1}{4\ln(h/\hbar_0)}
\]

\[b_1 < 0, b_L > 0\]

\[
2 \left( \frac{h}{\hbar_0} \frac{2}{U} \sqrt{\frac{\pi}{e}} - \left( \frac{h}{\hbar_0} \right)^{-2/b_1} G^{-\frac{i\pi U}{4b_1}} - \left( \frac{h}{\hbar_0} \right)^{-2/b_L} G^{-\frac{i\pi U}{4b_L}} - \frac{h}{\pi^2 h_c} + \frac{1}{2} \right) \\
\frac{1}{4\ln(h/\hbar_0)}
\]

\[b_1 < 0, b_L < 0\]

By taking the limit $h \to 0$, the values of the phase shift $\delta_s$ given in the above are reduced to those of the case under zero magnetic field ($h = 0$). We recall that the phase shift $\delta_s$ under $h = 0$ are listed in Table I of §4.3.

For the non-half-filling and non-zero magnetic field case, the set of integral equations can not be reduced to scalar equations, and the calculation could be more complicated. In principle, however, it is possible to do it at least numerically.

6 Concluding Remarks

For the 1D Hubbard model under the general open-boundary conditions, we have derived the exact solutions by using the refraction equations of the open-boundary XXZ model, and then discussed the finite-size spectrum from the BCFT viewpoint.

The exact results obtained in this paper will be important in the study of the impurity effect in 1D interacting electrons. Furthermore, we can calculate exact formulas for the magnetic susceptibility and the specific heat of the open-boundary Hubbard model. The formulas are expressed in terms of the densities $\rho_s^L(k)$ and $\rho_c^L(v)$ of the rapidities discussed in the paper. The effect of the open-boundary conditions can be
derived by making use of the expansion $\rho_L = \rho + \tau/L + o(1/L)$. Thus we can evaluate the ‘Wilson ratio’ of the impurity, which should characterize the impurity effect of the 1D interacting electrons or the Tomonaga-Luttinger liquid. The details will be given in later papers.  

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Note: After submission of this work, we were informed that the same Bethe ansatz equations of the open-boundary Hubbard model with the boundary magnetic fields were also discussed independently by M. Shiroishi and M. Wadati in Ref. [35].

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7 Appendix A:

In this appendix, we give some steps to derive the Bethe ansatz equation for open boundary system.

First we consider one-particle state. The eigenstate can be assumed to be

\[ \Psi_1 = \sum_{x=1}^{L} f(x) c^\dagger_{x \sigma} |\text{vac} \rangle. \tag{A.1} \]

Applying the Hamiltonian (1.2) into this ansatz, one can obtain

\[
Ef(x) = -f(x+1) - f(x-1) + f(x)[\mu - \frac{\hbar}{2}(1 - 2M)], \quad 2 \leq x \leq L - 1
\]

\[
Ef(1) = -f(2) + f(1)[\mu - \frac{\hbar}{2}(1 - 2M) + p_{1\sigma}] \tag{A.2}
\]

\[
Ef(L) = -f(L-1) + f(L)[\mu - \frac{\hbar}{2}(1 - 2M) + p_{L\sigma}]
\]

We assume the wave function \( f(x) \) to be

\[ f(x) = A_{\sigma}(k)e^{ikx} - A_{\sigma}(-k)e^{-ikx} \tag{A.3} \]

From this ansatz and Equation (A.2), we have

\[
A_{\sigma}(k)\alpha_{\sigma}(-k) = A_{\sigma}(-k)\alpha_{\sigma}(k)
\]

\[
A_{\sigma}(k)\beta_{\sigma}(k) = A_{\sigma}(-k)\beta_{\sigma}(-k)
\]

\[ \alpha_{\sigma}(k) = 1 + p_{1\sigma}e^{-ik} \]

\[ \beta_{\sigma}(k) = (1 + p_{L\sigma}e^{-ik})e^{ik(L+1)} \tag{A.4} \]

The Compatibility of the above equation (A.5) gives the Bethe ansatz equation

\[
\frac{(1 + p_{1\sigma}e^{-ik})(1 + p_{L\sigma}e^{-ik})}{(1 + p_{1\sigma}e^{ik})(1 + p_{L\sigma}e^{ik})}e^{2ik(L+1)} = 1. \tag{A.5}
\]

The energy is given by \( E = -2\cos k + \mu - \hbar/2 \). We may choose \( A_{\sigma}(k) \) as \( \beta_{\sigma}(-k) \) up to a factor which is invariant under changing the sign of \( k \).

Next, let us consider the general eigenstates (2.1). Substituting the ansatz (2.1) and (2.2) into the eigenvalue equation, one can derive the energy (2.5) and the following
relations

\[ A_{\sigma_j \sigma_{j+1} \cdots k_p, k_{p+1}, \cdots} = \sum Y^j_{k_p, k_{p+1}} A_{\sigma_j' \sigma_{j+1}' \cdots (k_p', k_{p+1}', \cdots)} \] (A.6)

\[ A_{\sigma q_1 \cdots k_p} = U_{\sigma q_1} (k_p) A_{\sigma q_1 \cdots (k_p, \cdots)} \] (A.7)

\[ A_{\sigma q_1 \cdots k_p N} = V_{\sigma q_N} (-k_p N) A_{\sigma q_1 \cdots k_p N} \] (A.8)

where the operator \( Y \) is defined by

\[ Y^j_{k_p, k_{p+1}} = \frac{iU/2}{\sin k_{p+1} - \sin k_p + iU/2} I + \frac{iU/2}{\sin k_{p+1} - \sin k_p + iU/2} P^j_{k_p, k_{p+1}}. \] (A.9)

Using the relations (A.6)-(A.8), one can get the equation (2.3). The operator \( X \) is defined by \( X = PY \).

In order to diagonalize equation (2.3), we introduce the following operator \( T \) acting on the function \( IA \)

\[ T(\sin k_1) = tr_0 K_0^+(\sin k_1) L_0(\sin k_1, -\sin k_1) L_0(\sin k_1, -\sin k_2) \cdots L_0(\sin k_1, -\sin k_N) \]

\[ K_0^-(\sin k_1) L_0(\sin k_1, \sin k_N) \cdots L_0(\sin k_1, \sin k_2) L_0(\sin k_1, \sin k_1) \] (A.10)

where

\[ L_{0j}(\sin k_1, \sin k_j) = \frac{\sin k_1 - \sin k_j}{\sin k_1 - \sin k_j + iU/2} + \frac{iU/2}{\sin k_1 - \sin k_j + iU/2} P_{0j} \]

\[ K_0^+(\sin k) = \frac{2 \sin k + iU/2}{2 \sin k(2 \sin k + iU)} \text{diag.} \left( (2 \sin k + iU/2) U_+(k) - i(U/2) U_+(k) \right) \]

\[ K_0^-(\sin k) = \text{diag.} \left( V_+(k), V_+(k) \right) \] (A.11)

In terms of the operator \( T(u) \) the equation \( (2.3) \) is given by the form

\[ T(\sin k_{p1}) \bar{A}(k_{p1}, \cdots, k_{pN}) = \bar{A}(k_{p1}, \cdots, k_{pN}), \] (A.12)

where the eigenvalue is given by 1. We note that if \( T(u)T(v) = T(v)T(u) \) for any \( u \) and \( v \), then the transfer matrix can be diagonalized, i.e., the model is integrable.
From the solution of the reflection equation of the XXX model \cite{18} we find that $T$’s commute (the reflection equation) if the $U$’s and $V$’s satisfy the following relations

\[
V^\dagger(k)V(-k) = \frac{\zeta_+ + \sin k}{\zeta_- - \sin k},
\]

\[
U^\dagger(k)U(-k) = \frac{\zeta_+ + \sin k}{\zeta_- - \sin k}.
\]

Making use of the expression of the eigenvalue of the inhomogeneous transfer matrix for the XXX model with open boundary condition \cite{18}, we calculate the eigenvalue $\Lambda(\sin k)$ of $T(\sin k)$

\[
\Lambda(\sin k) = \frac{(2 \sin k + iU/2)U^\dagger(k)V^\dagger(k)}{(2 \sin k + iU)(\zeta_+ - \sin k)(\zeta_- - \sin k)}\bar{\Lambda}(\sin k))
\]

\[
\bar{\Lambda}(\sin k) = \frac{2 \sin k + iU}{2 \sin k + iU/2}(\zeta_+ + \sin k)\Delta_+(\sin k + iU/4)
\]

\[
\times \prod_{m=1}^M \frac{(\sin k - v_m - iU/4)(\sin k + v_m + iU/4)}{(\sin k - v_m + iU/4)(\sin k + v_m + iU/4)} - \frac{1}{2 \sin k + iU/2}(\sin k - \zeta_+ + iU/4)\Delta_- (\sin k + iU/4)
\]

\[
\prod_{m=1}^M \frac{(\sin k - v_m + i3U/4)(\sin k + v_m + i3U/4)}{(\sin k - v_m + iU/4)(\sin k + v_m + iU/4)}
\]

where

\[
\Delta_+(x) = (\zeta_+ + x - iU/4)\delta_+(x)\phi(x - iU/4)
\]

\[
\Delta_-(x) = (\zeta_- - x - iU/4)\delta_+(x)\phi(x - iU/4)
\]

\[
\delta_+(x) = \prod_{j=1}^N (x - \sin(k_j) + iU/4)
\]

\[
\delta_-(x) = \prod_{j=1}^N (x - \sin(k_j) - iU/4)
\]

\[
\phi^{-1}(x) = \prod_{j=1}^N (x - \sin(k_j) + iU/2)(-x - \sin(k_j) - iU/2)
\]

From the condition that $\Lambda(\sin k_p) = 1$ and the Bethe ansatz equation for the XXX model with open boundary, we obtain the Bethe ansatz equations (2.6) and (2.7) for the Hubbard model under the open boundary conditions.

We make some comments on the general eigenstates. (i) The number $N$ of particles should satisfy $N \leq L$. This is the condition for the existence of such configurations.
that have no overlap: \( x_{q_1} < \cdots < x_{q_N} \). The existence is important when we consider the connection between two different regions of ordering \( x_{q_1} \cdots < x_{q_N} \) and \( x_{q'_1} \cdots < x_{q'_N} \). (ii) For the region \( x_{q_1} \leq \cdots \leq x_{q_N} \) for \( Q \in S_N \) we may consider the wave function \( \tilde{f} \) with the ordering of the fermions given in the following

\[
\Psi_{NM} = \sum f_{\sigma_{q_1} \cdots \sigma_{q_N}} (x_{q_1}, \cdots, x_{q_N}) \epsilon_Q c_{x_{q_1} \sigma_{q_1}}^\dagger \cdots c_{x_{q_N} \sigma_{q_N}}^\dagger |\text{vac}\rangle \quad (A.16)
\]

where \( \epsilon_Q = \exp\{i\pi/2 \sum_{j=1}^L j (\sigma_{q_j} - \sigma_j) \} \).

8 Appendix B:

We introduce the following notation

\[
k_{-j} = -k_j \quad v_{-m} = -v_m \quad (k_0 = v_0 = 0). \tag{B.1}
\]

We define

\[
Z_L^c(k) = \frac{1}{\pi} \left\{ k + \frac{1}{2L} \sum_{m=-M}^M 2 \tan^{-1} \left( \frac{\sin k - v_m}{U/4} \right) + \frac{1}{2L} P_0(k) \right\} \tag{B.2}
\]

\[
Z_L^v(v) = \frac{1}{\pi} \left\{ \frac{1}{2L} Q_0(v) + \frac{1}{2L} \sum_{j=-N}^N 2 \tan^{-1} \left( \frac{v - \sin k_j}{U/4} \right) - \frac{1}{2L} \sum_{m=-M}^M 2 \tan^{-1} \left( \frac{v - v_m}{U/2} \right) \right\} \tag{B.3}
\]

where

\[
P_0(k) = \phi(k) + \psi(k) - 2 \tan^{-1} \frac{\sin k}{U/4}
\]

\[
Q_0(v) = \Gamma_+(v) + \Gamma_-(v) - 2 \tan^{-1} \frac{v}{U/4} + 2 \tan^{-1} \frac{v}{U/2}. \tag{B.4}
\]

We recall that

\[
\phi(k_j) = \frac{1}{i} \log \frac{1 + p_{1\uparrow} e^{-ik_j}}{1 + p_{1\uparrow} e^{ik_j}}, \quad \psi(k_j) = \frac{1}{i} \log \frac{p_{L\uparrow} + e^{ik_j}}{p_{L\uparrow} + e^{-ik_j}}
\]

\[
\Gamma_\pm(v) = \frac{1}{i} \log \frac{U/4 + i(\zeta_\pm - v)}{U/4 + i(\zeta_\pm + v)}.
\]
With these notations, the Bethe ansatz equations (2.6) and (2.7) are expressed as

\[ Z^c_L(k_j) = \frac{I_j}{L}, \quad Z^s_L(v_m) = \frac{J_m}{L} \] (B.5)

We note that \( Z^c_L(k) \) and \( Z^s_L(v) \) are odd functions: \( Z^c_L(-k) = -Z^c_L(k) \) and \( Z^s_L(-v) = -Z^s_L(v) \).

Let us denote the maxima of \( \{I_j\} \) and \( \{J_m\} \) by \( I_{\text{max}} \) and \( J_{\text{max}} \), respectively. Then we define \( k^+ \) and \( v^+ \) by

\[ Z^c_L(k^+) = \frac{I_{\text{max}} + 1/2}{L}, \quad Z^s_L(v^+) = \frac{J_{\text{max}} + 1/2}{L} \] (B.6)

We define the density functions \( \rho^c_L(k) \) and \( \rho^s_L(v) \) by the derivatives of \( Z^c_L(k) \) and \( Z^s_L(v) \), respectively. Then the parameters \( k^+ \) and \( v^+ \) are related to \( N \) and \( M \) by

\[ \int_{-k^+}^{k^+} \rho^c_L(k) dk = \frac{2N + 1}{L}, \quad \int_{-v^+}^{v^+} \rho^s_L(v) dv = \frac{2M + 1}{L}. \] (B.7)

Using the Euler-MacLaurin formula

\[ \frac{1}{L} \sum_{n=n_1}^{n_2} \frac{n}{L} f(x) \simeq \int_{(n_1-1/2)/L}^{(n_2+1/2)/L} f(x) dx + \frac{1}{24L^2} \left[ f'(\frac{n_1 - 1/2}{L}) - f'(\frac{n_2 + 1/2}{L}) \right], \] (B.8)

the density functions under the large-\( L \) limit can be written as

\[
\rho^c_L(k) = \frac{1}{\pi} \left\{ 1 + \frac{1}{2L} P_0'(k) + \frac{1}{2} \int_{-v^+}^{v^+} K_1(\sin k - v) \rho^s_L(v) dv \cos k 
+ \frac{\cos k}{48L^2} \left( \frac{K_1'(\sin k + v^+)}{\rho^s_L(-v^+)} - \frac{K_1'(\sin k - v^+)}{\rho^s_L(v^+)} \right) \right\} \tag{B.9}
\]

\[
\rho^s_L(v) = \frac{1}{2\pi} \left\{ \frac{1}{L} Q_0(v) + \frac{\cos k^+}{24L^2} \left( \frac{K_1'(v - \sin k^+)}{\rho^c_L(k^+)} - \frac{K_1'(v + \sin k^+)}{\rho^c_L(-k^+)} \right) 
+ \frac{1}{24L^2} \left( \frac{K_2'(v + v^+)}{\rho^c_L(-v^+)} - \frac{K_2'(v - v^+)}{\rho^c_L(v^+)} \right) 
+ \int_{-k^+}^{k^+} K_1(v - \sin k) \rho^c_L(k) dk + \int_{-v^+}^{v^+} K_2(v - v') \rho^s_L(v') dv' \right\} \tag{B.10}
\]
In the above derivation we have used the fact that $k_j \neq 0$ for $j \neq 0$, and $v_m \neq 0$ for $m \neq 0$. In eqs. (B.9) and (B.10) the kernels are given by

\[
K_1(x) = \frac{2U/4}{(U/4)^2 + x^2}, \quad K_2(x) = \frac{2U/2}{(U/2)^2 + x^2}
\]  

(B.11)

For notational convenience, we introduce an integral matrix operator $\mathbf{K}$ for a two-component function $Y(k, v) = (Y^c(k), Y^s(v))^T$ as:

\[
\mathbf{K}(k, v|k', v')Y(k', v') =
\begin{pmatrix}
0 & \cos k \int_{v+}^{v-} K_1'(\sin k - v')Y^s(v')dv' \\
\int_{k+}^{k-} K_1(v - \sin k')Y^c(k')dk' & -\int_{v+}^{v-} K_2(v - v')Y^s(v')dv'
\end{pmatrix}.
\]  

(B.12)

We also introduce its transpose $\mathbf{K}^T$

\[
\mathbf{K}^T(k, v|k', v') = \frac{1}{2\pi} \begin{pmatrix}
0 & \int_{v-}^{v+} K_1'\sin k - v'dv' \\
\int_{k+}^{k-} K_1(v - \sin k')\cos k'dk' & -\int_{v-}^{v+} K_2(v - v')dv'
\end{pmatrix}.
\]  

(B.13)

Then the functional equations of the densities can be written as equation (3.3). Here the densities $\rho^0, \tau^0, \sigma^0_1$ and $\sigma^0_2$ are given in the following.

\[
\rho^0(k, v) = \begin{pmatrix}
\frac{1}{\pi} \\
0
\end{pmatrix}
\]

\[
\tau^0(k, v) = \begin{pmatrix}
\frac{1}{2\pi}P_0'(k) \\
\frac{1}{2\pi}Q_0'(v)
\end{pmatrix}
\]

\[
\sigma^0_1(k, v) = \begin{pmatrix}
0 \\
\frac{1}{2\pi}[K_1'(v - \sin k^+) - K_1'(v + \sin k^+)]
\end{pmatrix}
\]

\[
\sigma^0_2(k, v) = \begin{pmatrix}
0 \\
\frac{1}{2\pi}[K_1'(\sin k - v^+) - K_1'(\sin k + v^+)] \\
-\frac{1}{2\pi}[K_2'(v - v^+) - K_2'(v + v^+)]
\end{pmatrix}
\]  

(B.14)

Let us consider the integral equations

\[
Y(k, v) = Y^0(k, v) + \mathbf{K}(k, v|k', v')Y(k', v').
\]  

(B.15)
Then the formal solution to (B.15) can be represented as
\[ Y(k, v) = \sum_{n=0}^{\infty} (K)^n(k, v, |k', v')Y^0(k', v') \] (B.16)

Thus, for the initial densities \( \rho^0, \tau^0, \sigma_1^0 \) and \( \sigma_2^0 \) we have the formal solutions \( \rho, \tau, \sigma_1 \) and \( \sigma_2 \), respectively.

We now define the dressed energy \( e(k, v) \) by
\[ e(k, v) = e^0(k, v) + K^T(k, v|k', v')e(k', v'). \] (B.17)

The bulk energy density \( e_\infty \) of the infinite system can be written
\[ e_\infty(k^+, v^+) = (e^0(k, v), \rho) = (e(k, v), \rho^0). \] (B.18)

Notice that the energy \( e_\infty \) depends on the parameters \( k^+ \) and \( v^+ \).

We now consider the parameters \( k_0^* \) and \( v_0^* \) denoting the Fermi surfaces of the ground state of the infinite system. They are defined by the following
\[ \frac{\partial e_\infty(k^+, v^+)}{\partial k^+} \bigg|_{k^+ = k_0^*, v^+ = v_0^*} = 0, \quad \frac{\partial e_\infty(k^+, v^+)}{\partial v^+} \bigg|_{k^+ = k_0^*, v^+ = v_0^*} = 0. \] (B.19)

We note that as for the periodic case, (B.19) can be reduced to the condition that the dressed energy should vanish at the Fermi surfaces: \( e^c(k_0^*) = e^s(v_0^*) = 0 \). Thus the energy for the low-excited states (3.6) are asymptotically expanded upto \( O(1/L^2) \) as
\[ e_L = e(k_0^*, v_0^*) + \frac{1}{L}[1 - \mu_s - h_s + (e^0, \tau)|_g] \]
\[ + \frac{1}{L^2} \epsilon_1(k_0^*, v_0^*)\left\{ \frac{L^2}{2} (k^+ - k_0^*)^2 \rho^c(k_0^*, v_0^*)^2 - \frac{1}{24} \right\} \]
\[ + \frac{1}{L^2} \epsilon_2(k_0^*, v_0^*)\left\{ \frac{L^2}{2} (v^+ - v_0^*)^2 \rho^s(k_0^*, v_0^*)^2 - \frac{1}{24} \right\}. \] (B.20)

We now express (B.20) in terms of the variables \( N \) and \( M \). Here we recall the definitions of \( n_0^c \) and \( n_0^s \) in §3. Then we can represent the \( k^+ - k_0^* \) and \( v^+ - v_0^* \) in (B.20) in terms of the numbers of electrons
\[ \xi_{11} 2\rho_\infty(k_0^*)(k^+ - k_0^*) + \xi_{12} 2\rho_\infty(v_0^*)(v^+ - v_0^*) = \frac{1}{L} (2N + 1 - 2Ln_0^c - \int_{-k_0^*}^{k_0^*} \tau^c(k)dk) \]
\[ \xi_{21} 2\rho_\infty(k_0^*)(k^+ - k_0^*) + \xi_{22} 2\rho_\infty(v_0^*)(v^+ - v_0^*) = \frac{1}{L} (2M + 1 - 2Ln_0^s - \int_{-v_0^*}^{v_0^*} \tau^s(v)dv) \] (B.21)

From the above equations the finite-size correction (3.15) is readily derived.