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A gapless charge mode induced by the boundary states in the half-filled Hubbard open chain

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Abstract. We discuss the ground state and some excited states of the half-filled Hubbard model defined on an open chain with L sites, where only one of the boundary sites has a different value of chemical potential. We consider the case when the boundary site has a negative chemical potential $-p$ and the Hubbard coupling U is positive. By an analytic method we show that when p is larger than the transfer integral some of the ground-state solutions of the Bethe ansatz equations become complex-valued. It follows that there is a 'surface phase transition' at some critical value p_c; when $p < p_c$ all the charge excitations have the gap for the half-filled band, while there exists a massless charge mode when $p > p_c$.

The Mott-insulator transition is a fundamental phenomenon where the strong correlation among electrons plays an essential role. The existence of the insulating phase, which we call the Mott insulator, cannot be explained within the standard framework of the band theory. For the one-dimensional (1D) Hubbard model, it is well known that under the periodic boundary condition the charge gap exists only for the positive Hubbard coupling $U > 0$ and at half-filling [1]. Near the transition point, however, the system shows quite nontrivial many-body effects [2–5]. For instance, the effective mass diverges at half-filling for the Hubbard ring [2].

In order to investigate many-body effects near the transition point very precisely, let us consider a Hubbard chain in which only one site has a different chemical potential. With the local chemical potential we can effectively change the number of electrons (or holes) of the Mott insulator, *infinitesimally*. Let us assume L electrons in the Hubbard chain with L sites. The system is divided into two parts; a 'surface' part consisting of only the site with the local chemical potential, and a 'bulk' part of the other $L-1$ sites. When the local potential is zero, the number of electrons in the bulk part is given by $L-1$; when it is very large, no electron should occupy the surface site and hence all the electrons should be in the bulk part. Thus, by controlling the parameter, the effective number of electrons in the bulk part ($L-1$ sites) can be changed continuously from $L-1$ to L. The property of the

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electrons in the bulk part is unique: if we consider a standard closed system, the electron number will be given by some integer and cannot increase or decrease infinitesimally.

In this paper, we consider the Hubbard system defined on an open chain, where one of the two boundary sites is chosen as the surface site. We discuss how the half-filled ground state changes under the local chemical potential. We derive complex ground-state solutions of the Bethe ansatz equations by an analytic approach. We find them explicitly for some finite-size systems, solving the Bethe ansatz equations numerically. Then, we calculate the energy of the ground state with the complex solutions, analytically. It is our hope that the study of this paper might shed some light on some new aspects of the many-body effects of the Hubbard system near the metal–insulator transition.

The study of this paper could be related to some real 1D systems such as Cu–O chain [6] and quantum or atomic wires [7, 8]. The open-boundary 1D Hubbard system with the boundary chemical potential could be realized in some 1D Hubbard system in reality, where the local chemical potential may play the role of a nonmagnetic impurity or a bias potential.

Let us introduce the 1D Hubbard Hamiltonian under the open-boundary condition, in which only the first site has the local chemical potential $-p$.

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

Here $c_{j,\sigma}$ and $n_{j,\sigma}$ stand for the annihilation and number operators of electron located at the jth site with spin σ, respectively. We recall that U denotes the Hubbard interaction and t the transfer integral. Hereafter we set $t = 1$. The Bethe ansatz equations for the 1D Hubbard model have been discussed under some different cases of open-boundary conditions [9–12] (see also [13]). In this paper we discuss the open-boundary Hubbard system with $p \geqslant 0$.

For N electrons with M down spins, the roots of the Bethe ansatz equations are given by momenta (charge rapidities) k_j for $j = 1$ to N and rapidities (spin rapidities) v_m for $m = 1$ to M. With some functions $Z_L^c(k)$ and $Z_L^s(v)$, the Bethe ansatz equations can be written as

$$Z_L^c(k_j) = I_j/L \qquad \text{for } j = 1, \ldots, N \qquad Z_L^s(v_m) = J_m/L \qquad \text{for } v = 1, \ldots, M. \qquad (2)$$

Here the quantum numbers I_j and J_m are given by some integers.

Let us consider the half-filled band under the boundary chemical potential, where $N = L$ and $M = L/2$. Hereafter we assume that L is even. We consider analytic continuations of the functions $Z_L^c(k)$ and $Z_L^s(v)$ with respect to the parameter p. Let us introduce an adiabatic hypothesis that the quantum numbers I_j and J_m should be constant when we continuously change the parameter p. Under the hypothesis, all the solutions of the Bethe ansatz equations can be labelled by their quantum numbers. When $p = 0$, we can order the ground-state roots k_j's and v_m's such that $I_j = j$ for $1 \leqslant j \leqslant L$ and $J_m = m$ for $1 \leqslant m \leqslant L/2$. The hypothesis is consistent with our analytic arguments and numerical results. Thus, for any value of p, the quantum numbers of momentum k_j and rapidity v_m are given by j and m, respectively.

We now consider the Bethe ansatz equations more explicitly. Let us denote by $I_{\max}$ ($I_{\min}$) the largest (smallest) integer of the quantum numbers of real momenta over all possible excitations and by $J_{\max}$ ($J_{\min}$) that of real rapidities. Then, the set Δ_{re}^c (Δ_{re}^s) of all the possible quantum numbers I_j's (J_m's) for real momenta (rapidities) are given by

$$\Delta_{\mathrm{re}}^c = \{I_{\min}, I_{\min}+1, \ldots, I_{\max}\} \qquad (\Delta_{\mathrm{re}}^s = \{J_{\min}, J_{\min}+1, \ldots, J_{\max}\}). \qquad (3)$$

Let us write by Δ_{hole}^c (Δ_{hole}^s) the set of the quantum numbers of holes of real momenta (rapidities) in the ground state. Then, the set of the quantum numbers of the real momenta (rapidities) for the ground state is given by $\Delta_g^c = \Delta_{\mathrm{re}}^c - \Delta_{\mathrm{hole}}^c$ ($\Delta_g^s = \Delta_{\mathrm{re}}^s - \Delta_{\mathrm{hole}}^s$). Let us

denote by $I^g_{\max}$ ($J^g_{\max}$) the largest integer of the set Δ^c_g (Δ^s_g). Then, $I^g_{\max} \leqslant I_{\max}$, in general. We introduce the symbol $\Delta^c_{\rm im}$ ($\Delta^s_{\rm im}$) for the set of the quantum numbers for complex-valued momenta (rapidities) in the ground state. In terms of the symbols, the functions $Z^c_L(k)$ and $Z^s_L(v)$ for the ground state are written as follows:

$$\begin{aligned} Z^c_L(k) &= \frac{2k}{2\pi} + \frac{1}{L}\sum_{n\in\Delta^s_g}\sum_{r=\pm1}\theta_1(\sin k - r v_n) + \frac{1}{L}z^c_B(k) \\ Z^s_L(v) &= \frac{1}{L}\sum_{j\in\Delta^c_g}\sum_{r=\pm1}\theta_1(v - r\sin k_j) - \frac{1}{L}\sum_{n\in\Delta^s_g}\sum_{r=\pm1}\theta_2(v - r v_n) + \frac{1}{L}z^s_B(v) \end{aligned} \tag{4}$$

where the functions $z^c_B(k)$ and $z^s_B(v)$ are given by

$$\begin{aligned} z^c_B(k) &= \frac{2k}{2\pi} - \frac{1}{2\pi {\rm i}}\log\left(\frac{1+p{\rm e}^{{\rm i}k}}{1+p{\rm e}^{-{\rm i}k}}\right) + \sum_{m\in\Delta^s_{\rm im}}\sum_{r=\pm1}\theta_1(\sin k - r v_m) \\ z^s_B(v) &= \theta_1(v) + \sum_{j\in\Delta^c_{\rm im}}\sum_{r=\pm1}\theta_1(v - r\sin k_j) - \sum_{m\in\Delta^s_{\rm im}}\sum_{r=\pm1}\theta_2(v - r v_m). \end{aligned} \tag{5}$$

Here, the functions $\theta_n(x)$ have been defined by $\theta_n(x) = 2\tan^{-1}(x/(nu))/(2\pi)$, where u is given by $u = U/4$. An outline of the derivation of the Bethe ansatz equations is given in appendix A.

When p is larger than some critical values of p, some of the ground-state solutions become complex-valued. The number of complex roots is different for four regions of p, which are divided by the critical values p_{cj}'s. They are given by $p_{c1} = 1$, $p_{c2} = u + \sqrt{1+u^2}$, $p_{c3} = 2u + \sqrt{1+4u^2}$. Let us introduce some notation. We define symbol κ by $\kappa = \log|p|$ for $p > 0$ and $p < 0$. We also define α by $\alpha = \sinh\kappa/u$ for $p > 0$ and $p < 0$. The notation of the critical points is summarized as $p_{cj} = (j-1)u + \sqrt{1+(j-1)^2u^2}$ for $j = 1, 2, 3$. If a set Δ is empty, we denote it by $\Delta = \phi$. Then, the sets of quantum numbers are given by the following.

(1) For $0 < p < p_{c1}$, we have no boundary solutions. The sets of quantum numbers are given by

$$\Delta^c_g = \{1, 2, \ldots, L\} \qquad \Delta^s_g = \{1, 2, \ldots, L/2\}$$
$$\Delta^c_{\rm im} = \Delta^s_{\rm im} = \Delta^c_{\rm hole} = \Delta^s_{\rm hole} = \phi.$$

The $I_{\min}$'s are given by the following

$$I_{\min} = 1 \qquad I_{\max} = L \qquad J_{\min} = 1 \qquad J_{\max} = L/2.$$

(2) For $p_{c1} < p < p_{c2}$ ($0 < \alpha < 1$), we have a complex-valued momentum k_L given by

$$k_L = \pi + {\rm i}\kappa - {\rm i}\delta_L. \tag{6}$$

The sets of quantum numbers are given by

$$\Delta^c_g = \{1, \ldots, L-1\} \qquad \Delta^s_g = \{1, 2, \ldots, L/2\}$$
$$\Delta^c_{\rm im} = \{L\} \qquad \Delta^s_{\rm im} = \Delta^c_{\rm hole} = \Delta^s_{\rm hole} = \phi.$$

The $I_{\min}$'s are given by the following:

$$I_{\min} = 1 \qquad I_{\max} = L-1 \qquad J_{\min} = 1 \qquad J_{\max} = L/2.$$

(3) For $p_{c2} < p < p_{c3}$ ($1 < \alpha < 2$), we have the complex momentum k_L and the complex rapidity v_1 given by

$$\begin{aligned} k_L &= \pi + {\rm i}\kappa - {\rm i}\delta_L \\ v_1 &= {\rm i}(\alpha - 1)u + {\rm i}\eta_1. \end{aligned} \tag{7}$$

The sets of quantum numbers are given by

$$\Delta_g^c = \{1, \ldots, L-1\} \qquad \Delta_g^s = \{2, \ldots, L/2\}$$
$$\Delta_{\rm im}^c = \{L\} \qquad \Delta_{\rm im}^s = \{1\} \qquad \Delta_{\rm hole}^c = \Delta_{\rm hole}^s = \phi.$$

The $I_{\rm min}$'s are given by the following:

$$I_{\rm min} = 1 \qquad I_{\rm max} = L-1 \qquad J_{\rm min} = 2 \qquad J_{\rm max} = L/2.$$

(4) For $p_{c3} < p$ $(2 < \alpha)$, we have the following three complex roots k_1, k_L and v_1

$$\begin{aligned} k_1 &= {\rm i}\log\left((\alpha-2)u + \sqrt{(\alpha-2)^2u^2+1}\right) + {\rm i}\delta_1 \\ k_L &= \pi + {\rm i}\kappa - {\rm i}\delta_L \\ v_1 &= {\rm i}(\alpha-1)u + {\rm i}\eta_1. \end{aligned} \tag{8}$$

We call them a *boundary* $k-\Lambda$ *string*. The sets of quantum numbers are given by

$$\Delta_g^c = \{2, 3, \ldots, L-1\} \qquad \Delta_g^s = \{2, 3, \ldots, L/2\}$$
$$\Delta_{\rm im}^c = \{1, L\} \qquad \Delta_{\rm im}^s = \{1\} \qquad \Delta_{\rm hole}^c = \{L\} \qquad \Delta_{\rm hole}^s = \phi.$$

The $I_{\rm min}$'s are given by the following:

$$I_{\rm min} = 2 \qquad I_{\rm max} = L \qquad J_{\rm min} = 2 \qquad J_{\rm max} = L/2.$$

We note that when $p > p_{c3}$, a hole of real momenta appears in the half-filled ground state at $I = L$; $I_{\rm max}^g = L-1$ and $I_{\rm max} = L$ when $p > p_{c3}$. We also note that δ_1, δ_L and η_1 are exponentially small except for some neighbourhoods of the critical points. For instance, we can show $\delta_1 = {\rm O}(p^{-2L})$ for $p_{c1} < p < p_{c2}$. The quantities δ_L, δ_1 and η_1 are explicitly evaluated in appendix B.

For the case when $p < 0$, some complex boundary solutions have been discussed for the 1D Hubbard model under the open-boundary conditions [14–16], where the quantum numbers of the complex rapidities k_1', k_2' and v_1' correspond to $I_1 = 1$, $I_2 = 2$ and $J_1 = 1$, respectively. Furthermore, when the bandwidth $4t$ is very large and the electron density N/L is very small, the boundary solutions k_1', k_2' and v_1' for the case of $p < 0$ can correspond to the boundary solutions of the 1D interacting spin-$\frac{1}{2}$ Fermi system, which had been discussed in [17] (see also appendix B).

For the half-filling case, the ground-state energy for $p > 0$ is related to that of $p < 0$ through the particle–hole transformation, which will be discussed in appendix C. For instance, the energy of the ground state for $p > p_{c3}$ with the boundary solutions k_L, k_1 and v_1, is transformed into that of $p < -p_{c3}$ with k_1', k_2' and v_1'. However, it seems quite nontrivial how the two sets of the charge rapidities for the two cases of $p > 0$ and $p < 0$ could be related to each other (see also appendix C).

Let us show that momentum k_L which is real-valued when $p < p_{c1}$ becomes complex-valued when $p > p_{c1}$. First, we note that when k is real and $|\pi - k| \ll 1$, we have

$$\frac{1}{2\pi{\rm i}}\log\left(\frac{1+p{\rm e}^{{\rm i}k}}{1+p{\rm e}^{-{\rm i}k}}\right) = H(p-p_{c1}) + \frac{2}{2\pi}\tan^{-1}\left(\frac{p\sin(\pi-k)}{1-p\cos(\pi-k)}\right) \tag{9}$$

where $H(x)$ denotes the Heaviside step-function: $H(x) = 0$ for $x < 0$ and $H(x) = 1$ for $x > 0$. Suppose that momentum k_L be real even when $p > 1$. Since k_L is close to π, we have $Z_L^c(k_L) = k_L/\pi + z_B^c(k_L)/L$. It follows from (9) that the value of $z_B^c(k_L)$ for $p > 1$ is by 1 smaller than that of the case when $p < 1$: $z_B^c(k_L) = k_L/\pi - 1 + {\rm O}(1/L)$ for $p > 1$. Thus, we have $I_L/L = k_L/\pi + (k_L/\pi - 1)/L + {\rm O}(1/L^2)$, which leads to $k_L = \pi + {\rm O}(1/L^2)$ for $I_L = L$. However, when $k = \pi$ the wavefunction should vanish under the open-boundary condition. Thus, we arrive at an inconsistency. Therefore, the momentum k_L should be complex-valued when $p > 1$.

We can show that v_1 becomes imaginary when $p > p_{c2}$. Let us take the following branch of the logarithmic function: $-\mathrm{i}\log(e(x)) = \pi - 2\tan^{-1}(x)$, where $e(x)$ denotes $e(x) = (x+\mathrm{i})/(x-\mathrm{i})$. Then, we can show

$$\sum_{r=\pm 1} \theta_n(v + r\mathrm{i}\gamma u) = \begin{cases} \theta_{\gamma+n}(v) + \theta_{n-\gamma}(v) & \text{for } \gamma < n \\ \theta_{\gamma+n}(v) + 1 - \theta_{\gamma-n}(v) & \text{for } \gamma > n. \end{cases} \tag{10}$$

Applying the formula (10) with $\gamma = \alpha$ to the function $z_B^s(v)$, we can show that if we assume the smallest rapidity v_1 to be real, then it would be $\mathrm{O}(1/L^2)$ for $p > p_{c2}$, and also that therefore it should be imaginary when $p > p_{c2}$. In the same way with the rapidity v_1, using the formula (10) we can also show that momentum k_1 becomes imaginary when $p > p_{c3}$.

We can evaluate the largest and smallest integers of all the possible quantum numbers for real momenta in the following way. The function $Z_L^c(k)$ is monotonically increasing with respect to k, since the density of real momenta should be non-negative. We note that under the open-boundary condition, the Bethe ansatz wavefunction should vanish if there exists a momentum of $k = 0$ or π. Thus, the equations for $I_{\min}$ and $I_{\max}$ are given by

$$Z_L^c(0) = (I_{\min} - 1)/L \qquad Z_L^c(\pi) = (I_{\max} + 1)/L. \tag{11}$$

We determine $I_{\min}$ and $I_{\max}$ by solving equations (11). For instance, for the case when $0 \leqslant p < 1$, it is easy to see $Z_L^c(0) = 0$ and $Z_L^c(\pi) = (L+1)/L$, so that we obtain $I_{\min} = 1$ and $I_{\max} = L$.

For real rapidities, we can obtain $J_{\min}$ and $J_{\max}$ by applying the argument in [18]. It is easy to show that they satisfy the following equations:

$$Z_L^s(0) = (J_{\min} - 1)/L \qquad Z_L^s(\infty) = (J_{\max} + 1)/L. \tag{12}$$

Solving equations (12) we determine $J_{\min}$ and $J_{\max}$. For example, let us consider the case $p_{c2} < p < p_{c3}$. From equations (4) and (5) we can show $Z_L^s(\infty) = 1 + (1 - J_{\max})/L$. Thus, we obtain $J_{\max} = L/2$. We can discuss the maximal and minimal quantum numbers also for some excited states with boundary solutions, similarly. Some details are given in appendix D.

The new hole appears in the half-filled band, when $p > p_{c3}$. Therefore, there is a gapless mode of particle–hole excitations for the half-filled ground state under the open-boundary condition. Let us give an explanation. The quantum number of the hole is given by L for the ground state, while for the charge excited state it is given by an integer less than L. Thus, the charge excitation energy for the excited state where the quantum number of the hole is close to L (for example, $L-1$) becomes infinitesimally small when we take the thermodynamic limit $L \to \infty$. Here we have assumed that the charge excitation energy should be continuous with respect to the hole rapidity. Furthermore, the new hole is a consequence of the formation of the boundary $k - \Lambda$ string. We recall that the number of possible real momenta in the band is given by $L-1$, since $I_{\max} = L$ and $I_{\min} = 2$ when $p > p_{c3}$. We also recall that there are only $L-2$ real momenta in the wavefunction since we have two complex momenta k_1 and k_L. Thus, there should be one hole in the band.

We can explicitly calculate the energy E_L^{ex} of the charge excited state with the new hole, applying the method [19] of the finite-size correction as we shall see later. Let us denote by k_h the charge rapidity of the new hole. Then it is given by

$$E_L^{\mathrm{ex}} = E_L^g - 2e^c(k_h) + 2e^c(\pi) \tag{13}$$

where E_L^g denotes the ground-state energy for $p > p_{c3}$ and $e^c(k)$ is the dressed energy [19] for the half-filled band given by

$$e^c(k) = -\frac{A}{2} - \cos k - \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-u\omega} J_1(\omega)\cos(\omega \sin k)}{\omega \cosh u\omega}\,\mathrm{d}\omega. \tag{14}$$

The expression of the chemical potential A at the half-filling will be given later in (24). From the expression of the excited energy (13)† we see that the gap energy of the mode is of the order of $1/L^2$. Thus, by taking the thermodynamic limit $L \to \infty$, the gap energy vanishes. In this sense, we may call the mode gapless.

The three boundary complex solutions for $p > p_{c3}$ can be considered as a variant of $k-\Lambda$ string that was originally defined for the periodic Hubbard model. In fact, we can derive the expressions (8) of the boundary $k-\Lambda$ string from the viewpoint of classification of $k-\Lambda$ strings of length $n=1$. Details will be discussed in later papers.

Let us explicitly study for a finite-size system the behaviours of momenta and rapidities with respect to the boundary chemical potential. In figure 1, the flows of momenta and rapidities are plotted versus the parameter p for the eight-sited Hubbard Hamiltonian under the open boundary condition, where the roots are obtained numerically by solving the Bethe ansatz equations with $L = N = 8$ and $M = 4$. As far as the finite-size systems we have investigated are concerned, the numerical solutions are consistent with the following consequences of the analytic approach: the complex solutions are formed one-by-one at the critical points of the parameter p; there is a charge hole when $p > p_{c3}$. This is nontrivial. The analytic method should be valid only when the system size is very large. However, these important properties are already observed in such a small system as the case of $L = 8$.

Let us explain how we apply to our system the method [19] of the finite-size correction. We consider the Hamiltonian $\mathcal{H}' = \mathcal{H} - AN - h(N-2M)/2$ where A and h are the chemical potential and the uniform magnetic field, respectively. In order to define densities of the roots of the Bethe ansatz equations, we extend $Z_L^c(k)$ and $Z_L^s(v)$ into odd functions defined both on positive and negative values of their variables. For an illustration, we consider the density of real-valued rapidities. When $0 \leqslant p < p_{c2}$, we have $Z_L^s(0) = 0$ and the function $Z_L^s(v)$ itself can be simply extended into an odd function of v by $Z_L^s(-v) = -Z_L^s(v)$ for $v > 0$. We define rapidity with negative suffix by $v_{-m} = -v_m$ for $m = 1, \ldots, L/2$. Then, the density of the real rapidities is given by the derivative $\rho_L^s(v) = \mathrm{d}Z_L^s(v)/\mathrm{d}v$ for $-\infty < v < \infty$. When $p_{c2} < p$, however, the function does not vanish at the origin: $Z_L^s(0) = 1/L$. In this case, we introduce some shifts of the function and the variable $\tilde{Z}_L^s(v) = Z_L^s(v) - 1/L$ and $\tilde{v}_m = v_{m+1}$, respectively. We also introduce rapidity of negative suffix by $\tilde{v}_{-m} = -\tilde{v}_m$, for $m > 0$. Then, the Bethe ansatz equations are given by

$$\tilde{Z}_L^s(\tilde{v}_m) = \tilde{J}_m/L \qquad \text{for } m = -\tilde{J}_{\max}^g, \ldots, \tilde{J}_{\max}^g \tag{15}$$

where $\tilde{J}_m = m$ and $\tilde{J}_{\max}^g = J_{\max}^g - 1$. Then, we can safely define the density of rapidities by the derivative $\rho_L^s(\tilde{v}) = \mathrm{d}\tilde{Z}_L^s(\tilde{v})/\mathrm{d}\tilde{v}$.

Taking the derivatives of the Bethe ansatz equations together with some continuous limits, we can systematically derive a set of equations for the densities of the system with L sites. For the half-filled band under zero magnetic field, the set of equations for the densities up to $\mathrm{O}(1/L)$ is given in the following:

$$\begin{aligned}
\rho_L^c(k) &= \frac{1}{\pi} + \frac{1}{L}\tau^{c(0)}(k) + \cos k \int_{-\infty}^{\infty} a_1(\sin k - v)\rho_L^s(v)\,\mathrm{d}v + \mathrm{O}(1/L^2) \\
\rho_L^s(v) &= \frac{1}{L}\tau^{s(0)}(v) + \int_{-\pi}^{\pi} a_1(v - \sin k)\rho_L^c(k)\,\mathrm{d}k \\
&\quad - \int_{-\infty}^{\infty} a_2(v - v')\rho_L^s(v')\,\mathrm{d}v' + \mathrm{O}(1/L^2).
\end{aligned} \tag{16}$$

Here $a_n(x)$ is defined by $2\pi a_n(x) = (2nu)/(x^2 + (nu)^2)$. The boundary terms $\tau^{c(0)}(k)$

† Expression (13) can be derived from the formula (18) by replacing the hole momentum k_h^g of the ground state by that of the excited state.

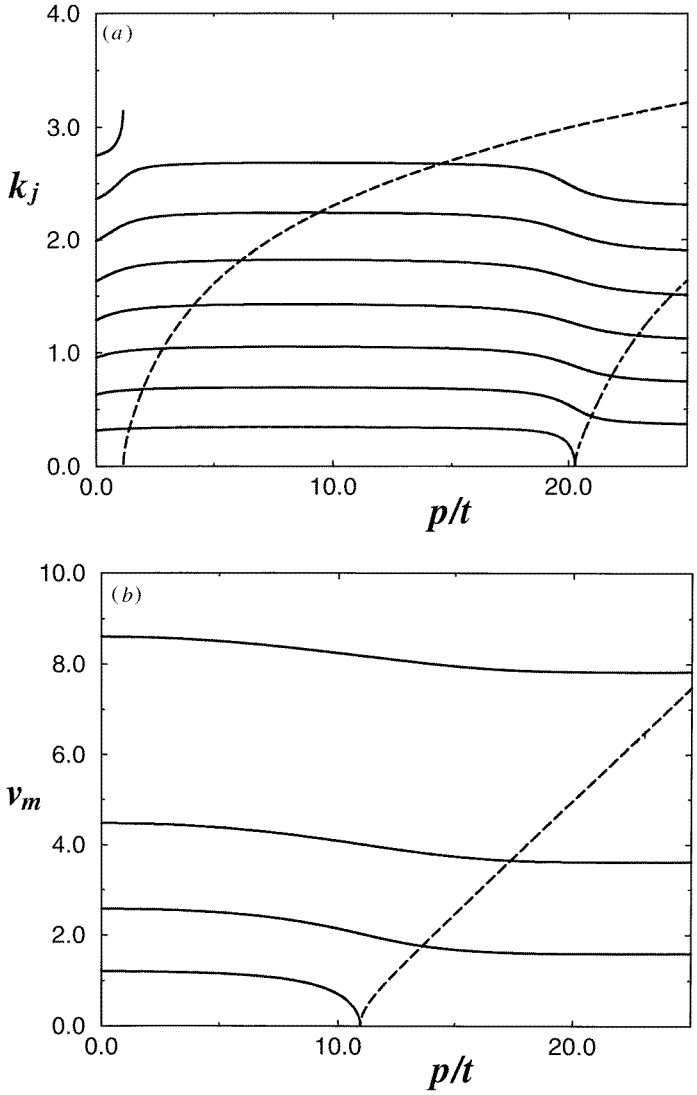

Figure 1. (*a*) Flow of momenta (or charge rapidities) as a function of boundary potential (p) for the one-dimensional open Hubbard model with eight sites at the half-filling ($N = L$) and $U = 20t$. Full curves represent real momenta. At $p = p_{c1} \sim t$, the largest charge rapidity approaches π and becomes complex, $\pi + \mathrm{i}\kappa$, whose complex part is given by the broken curve, for $p > p_{c1}$. Beyond $p = p_{c3} \sim U$, the smallest momentum becomes complex, $-\mathrm{i}\kappa'$, where κ' is represented by the chain curve. (*b*) Flow of rapidities (or spin rapidities) for the same system. Full curves represent real rapidities. At $p = p_{c2} \sim U/2$, the smallest rapidity becomes complex, $\mathrm{i}\chi$, where χ is given by the broken curve.

and $\tau^{s(0)}(v)$ in equations (16) are given by the derivatives of $P_0(k)/(2\pi)$ and $Q_0(v)/(2\pi)$, respectively, where they are related to $z_B^c(k)$ and $z_B^s(v)$ by

$$P_0(k)/2\pi = z_B^c(k) - \theta_1(\sin k) \qquad Q_0(v)/2\pi = z_B^s(v) - \theta_1(v) + \theta_2(v). \tag{17}$$

We now evaluate the ground-state energy E_L^g of the Hamiltonian $\mathcal{H}'$ at half-filling under

zero magnetic field. From equations (16) we have the following

$$E_L^g = -\sum_{j\in\Delta_g^c} 2\cos k_j - \sum_{j\in\Delta_{\rm im}^c} 2\cos k_j - AN$$
$$= Le_\infty + 1 + A/2 + (\boldsymbol{e}, \boldsymbol{\tau}^{(0)}) - \sum_{h\in\Delta_{\rm hole}^c} 2e^c(k_h^g)$$
$$- \sum_{j\in\Delta_{\rm im}^c} (A + 2\cos k_j) + {\rm O}(1/L) \tag{18}$$

where $\boldsymbol{\tau}^{(0)}(k, v) = (\tau^{c(0)}(k), \tau^{s(0)}(v))$ denotes the surface density, the symbol $\boldsymbol{e} = (e^c(k), e^s(v))$ denotes the dressed energy [19, 11]. We recall that k_h^g's denote the momenta of possible holes at the ground state. (For the ground state of $p > p_{c3}$, we have only one hole.) The inner product $(\boldsymbol{e}, \boldsymbol{\tau}^{(0)})$ is defined by the following [19, 11]:

$$(\boldsymbol{e}, \boldsymbol{\tau}^{(0)}) = \int_{-\pi}^{\pi} e^c(k)\tau^{c(0)}(k)\,{\rm d}k + \int_{-\infty}^{\infty} e^s(v)\tau^{s(0)}(v)\,{\rm d}v. \tag{19}$$

Let us define the surface energy $e_{\rm sur}$ of the system by the O(1) part of the ground-state energy. Then it is given in the following.

(1) For $0 < p < 1$,

$$e_{\rm con} + p - \sum_{n=0}^{\infty} p^{2n} \int_0^{\infty} \frac{2{\rm e}^{-u\omega} J_1(\omega) J_{2n}(\omega)}{\omega\cosh u\omega}\,{\rm d}\omega. \tag{20}$$

(2) For $1 < p < p_{c3}$,

$$e_{\rm con} + p - \int_0^{\infty} \frac{2{\rm e}^{-u\omega}\cosh(\omega\sinh\kappa) J_1(\omega)}{\omega\cosh u\omega}\,{\rm d}\omega + \sum_{n=1}^{\infty} \frac{1}{p^{2n}} \int_0^{\infty} \frac{2{\rm e}^{-u\omega} J_1(\omega) J_{2n}(\omega)}{\omega\cosh u\omega}\,{\rm d}\omega. \tag{21}$$

(3) For $p_{c3} < p$,

$$e_{\rm con} + 4u - A - \frac{1}{p} + \sum_{n=1}^{\infty} \frac{1}{p^{2n}} \int_0^{\infty} \frac{2{\rm e}^{-u\omega} J_1(\omega) J_{2n}(\omega)}{\omega\cosh u\omega}\,{\rm d}\omega. \tag{22}$$

Here the symbol $e_{\rm con}$ denotes the surface energy for $p = 0$, which is explicitly given by

$$e_{\rm con} = (1 - A/2) + 2\sqrt{1+u^2} - 2u - \int_0^{\infty} \frac{{\rm e}^{-2u\omega} J_1(\omega)}{\omega\cosh u\omega}\,{\rm d}\omega. \tag{23}$$

The chemical potential A at half-filling is given by

$$A = 2 - 2\int_0^{\infty} \frac{{\rm e}^{-u\omega} J_1(\omega)}{\omega\cosh u\omega}\,{\rm d}\omega. \tag{24}$$

Let us discuss the ground-state energy for the strong-coupling case. When $p > p_{c3}$, it becomes close to the energy of the first charge-excited state for $p = 0$. We compare the surface energy for $p = 0$ given by equation (20) with that of $p > p_{c3}$ given by equation (22). Then, the main part of the difference between them is given by $4u = U$, which is almost equivalent to the charge-gap energy $4u - 2A$ at $p = 0$. We note that when $u \gg 1$, we have $p_{c3} \gg 1$ and $u \gg A$.

Under the strong-coupling condition, the main part of the surface energy is given by the following: $p + e_{\rm con}$ when $1 \ll p < p_{c3}$ and $4u - 2A + e_{\rm con}$ when $p > p_{c3}$. From the calculation of the ground-state energy, we can evaluate the average number n_1 of electrons on the first site, since it is defined by $n_1 = \partial E_L/\partial p$. We find that $\partial E_L/\partial p \approx 1$ for $1 \ll p < p_{c3}$ and $\partial E_L/\partial p \approx 0$ for $p_{c3} < p$. This suggests that one hole should be localized at the surface site when $p > p_{c3}$. The result is consistent with the discussion over the complex boundary solutions that the half-filled ground state has gapless charge excitations when $p > p_{c3}$ since one hole appears in the band.

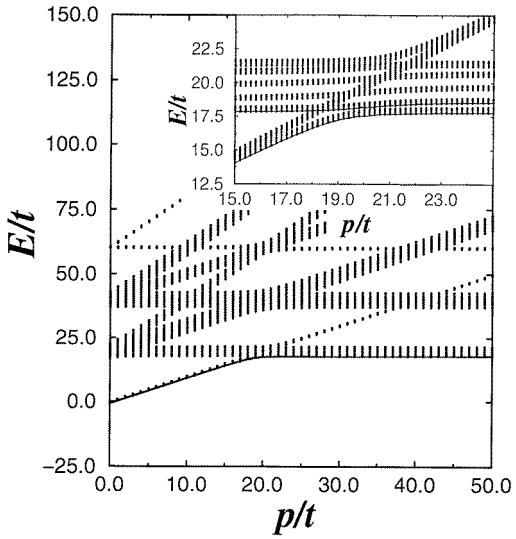

Figure 2. Spectral flow for the six-site open Hubbard chain at the half-filling with $U = 20t$ as a function of boundary potential p. Dots denote all of the eigenvalues for this system obtained by direct diagonalization. The lower full curve represents the ground-state energy given by the Bethe ansatz. The upper full curve corresponds to the first charge-excited state, which can be traced back from $p = p_{c3}$ to $p = 0$; at $p = 0$, it is the lowest level beyond the charge gap. Enlarged flow around the gap-closing transition point is depicted in the inset. Below a critical point (p_{c3}), a charge gap exists above the continuum of low-energy spin excitations.

Let us discuss the spectrum of a finite-size system numerically. The excited spectrum of the six-sited open Hubbard Hamiltonian with $U = 20t$ is obtained by the exact numerical diagonalization of the Householder method. The spectral flows with respect to the parameter p are depicted in figure 2, where we see that the energy levels of charge excitations become close to the ground-state energy at $p = p_{c3}$.

From figures 1 and 2, we have the following observations, respectively. (i) When $p > p_{c3}$ the first charge-excited state can be obtained by shifting the position of the hole in the band of real momenta k_j's; such shifting is equivalent to taking a different quantum number for the hole. (ii) The energy level of the first charge-excited state for $p > p_{c3}$ is identified with that of the lowest state above the charge gap for $p = 0$; we can trace the spectral flow of the excited state from $p = p_{c3}$ down to $p = 0$ in figure 2. From the analytic approach, the observation (ii) should hold due to the adiabatic hypothesis on the quantum numbers. From (i) and (ii), we can say that the characteristic properties of the energy spectrum discussed by the analytic method are also in common with that of the finite-size system. Thus, the spectrum of the six-sited system may illustrate that of thermodynamically large systems.

In this paper we have discussed the boundary solutions for the half-filled band when $p > 0$. We have shown that when $p > p_{c3}$ one mode of charge excitations has the gap energy of the order of $1/L^2$; we call it massless since the gap vanishes in the thermodynamic limit. By the method of the finite-size correction, we have calculated the ground-state energy and the excited energy of the massless mode. We note that it is not difficult to derive explicit formulae for the energies of other excitations. In fact, the whole spectrum shown in figure 2 can be explained analytically. Details will be given in the next paper [20].

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Appendix A

Let us briefly outline the derivation of the Bethe ansatz equations through the algebraic Bethe ansatz method for the open-boundary XXZ model given by Sklyanin. Some details can be found in [11] (see also [13]). We write the eigenstates for N electrons with M down-spins as

$$\Psi_{NM} = \sum f_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N) c^\dagger_{x_1\sigma_1}\ldots c^\dagger_{x_N\sigma_N}|vac\rangle. \tag{A.1}$$

Here, x_j and σ_j are the position and spin variables of the electrons, respectively. In the region $x_{Q1} \leqslant \cdots \leqslant x_{QN}$, we assume that the Bethe ansatz wavefunction f takes the form

$$f_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N) = \sum_P \epsilon_P A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{P1},\ldots,k_{PN}) \exp\left\{\mathrm{i}\sum_{j=1}^N k_{Pj}x_{Qj}\right\}. \tag{A.2}$$

Here the Q is an element of S_N, the permutation group of N particles, and P runs 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 employ the notation: $k_{-j} = -k_j$. The symbol ϵ_P denotes the sign of P; if the permutation is even, P makes $\epsilon_P = -1$ when odd number of k's are negative and $\epsilon_P = 1$ when even number of k's are negative. Let us introduce the vector $\boldsymbol{A}(k_{j_1},\ldots,k_{j_N})$ such that its element for entry $(Q1,\ldots,QN)$ is given by $A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{j_1},\ldots,k_{j_N})$. Here we note that the suffix $j_1,\ldots,j_N$ can be written as $P1,\ldots,PN$, respectively, by some P. Then, we can show that the consistency condition for the amplitudes $\boldsymbol{A}(k_{j_1},\ldots,k_{j_N})$ is given by the following

$$T(\sin k_{P1})\boldsymbol{A}(k_{P1},\ldots,k_{PN}) = \boldsymbol{A}(k_{P1},\ldots,k_{PN}). \tag{A.3}$$

Here $T(u)$ is the inhomogeneous transfer matrix of the open-boundary XXX model with N inhomogeneous parameters $\sin k_{P1},\ldots,\sin k_{PN}$ [11]. Let us denote the eigenvalue of the transfer matrix $T(u)$ by $\Lambda(u)$. Then, from the condition $\Lambda(\sin k_{P1}) = 1$ and the Bethe ansatz equations for the XXX model, the Bethe ansatz equations of the 1D open-boundary Hubbard model for the charge and spin parts are obtained, respectively.

Appendix B. Stability of the boundary solutions

Let us discuss explicitly the stability of the boundary solutions appearing in the ground state and some excited states, both for the cases $p > 0$ and $p < 0$. We recall some notation in the following. We have defined the symbols κ and α by $\kappa = |p|$ and $\alpha = \sinh\kappa/u$, respectively. The symbol p_{cj} is given by $p_{cj} = (j-1)u + \sqrt{1+(j-1)^2u^2}$ for some integer j; we note that $p = p_{cj}$ corresponds to $\alpha = j-1$.

Let us introduce a useful formula in the following

$$\theta_n(\mathrm{i}\gamma u - v) + \theta_n(\mathrm{i}\gamma u + v) = \frac{\mathrm{i}}{2\pi}\ln\left(\frac{(\gamma+n)^2u^2+v^2}{(\gamma-n)^2u^2+v^2}\right) \qquad \text{for } v > 0 \tag{B.1}$$

where $\gamma \geqslant 0$. We can show equation (B.1) by a similar method for the formula (10); we take the branch of the logarithmic function, and use the relations $\arg(\mathrm{i}(\gamma-n)u - v) = \arg(v - \mathrm{i}(\gamma-n)u) - \pi$ and $\arg(\mathrm{i}(\gamma+n)u - v) = \arg(v - \mathrm{i}(\gamma+n)) + \pi$.

For the case of $p > 0$, we may consider the three complex roots k_1, k_L and v_1 in the following regions:

$$\begin{aligned} &k_L = \pi + \mathrm{i}\kappa - \mathrm{i}\delta_L \qquad \text{for } \alpha > 0 \\ &v_1 = \mathrm{i}(\alpha-1)u + \mathrm{i}\eta_1 \qquad \text{for } \alpha > 1 \\ &k_1 = \mathrm{i}\log\left((\alpha-2)u + \sqrt{(\alpha-2)^2u^2+1}\right) + \delta_1 \qquad \text{for } \alpha > 2. \end{aligned} \tag{B.2}$$

We call the boundary solutions *stable* when δ_L, δ_1 and η_1 are very small. For convenience, we use symbols ϵ_1 and ϵ_L defined in the following:

$$\sin k_1 = \mathrm{i}(\alpha-1)u + \mathrm{i}\epsilon_1 \qquad \sin k_L = \mathrm{i}(\alpha-1)u + \mathrm{i}\epsilon_L \tag{B.3}$$

which are related to δ_1 and δ_L by

$$\epsilon_L = -\cosh\kappa \times \delta_L \qquad \epsilon_1 = \sqrt{(\alpha-2)^2u^2+1} \times \delta_1.$$

Let us give explicitly some evaluations of ϵ_L, η_1 and ϵ_1 for the case of $p > 0$. We assume that p is not close to any of the critical points p_{cj}'s. Then for the ground state and some excited states we can show the following.

(1) When there is only one boundary solution k_L, we have

$$\epsilon_L = \mathrm{O}(p^{-2L}). \tag{B.4}$$

(2) When there are two boundary solutions k_L and v_1 and when $u > 1$, we have

$$\begin{aligned} |\epsilon_L - \eta_1| &= \mathrm{O}\left(\left(\frac{\alpha}{2-\alpha}\right)^{-2N}\right) \\ |\epsilon_L| &= \mathrm{O}\left(\left(\frac{\alpha}{2-\alpha}\right)^{2N} p^{-2L}\right). \end{aligned} \tag{B.5}$$

(3) When there are three boundary solutions k_L, k_1 and v_1 and when $u > 1$, we have

$$\begin{aligned} |\epsilon_1 - \eta_1| &= \mathrm{O}(|z_1|^{2L}) \\ |\epsilon_L - \eta_1| &= \mathrm{O}\left(|z_1|^{2L}\left(\frac{\alpha}{\alpha-2}\right)^{-2N}\right) \\ |\epsilon_L| &= \mathrm{O}\left(|z_1|^{-2L}\left(\frac{\alpha}{\alpha-2}\right)^{2N} p^{-2L}\right). \end{aligned} \tag{B.6}$$

Here z_1 denotes the following

$$z_1 = \exp(\mathrm{i}k_1) = -(\alpha-2)u + \sqrt{(\alpha-2)^2u^2+1}.$$

It is easy to see that $|z_1| < 1$ for $\alpha > 2$.

We note that evaluations (B.4)–(B.6) can be applied for the half-filled ground-state solutions in the regions of $p_{c1} < p < p_{c2}$ $(0 < \alpha < 1)$, $p_{c2} < p < p_{c3}$ $(1 < \alpha < 2)$, and $p_{c3} < p$ $(2 < \alpha)$, respectively.

In the derivation of (B.5) and (B.6), we have assumed that $u > 1$. In fact, applying the formula (B.1) with $\gamma = \alpha - 1$, we can make the following approximation when $u > 1$:

$$\begin{aligned} \sum_j \sum_{r=\pm1} \theta(\mathrm{i}(\alpha-1)u - r\sin k_j) &= \sum_j \frac{\mathrm{i}}{2\pi} \ln\left(\frac{\alpha^2u^2+\sin^2 k_j}{(\alpha-2)^2u^2+\sin^2 k_j}\right) \\ &\approx \frac{\mathrm{i}N}{2\pi}\ln\left(\frac{\alpha^2}{(\alpha-2)^2}\right). \end{aligned} \tag{B.7}$$

We recall here that N is the number of electrons. The approximation (B.7) may not be effective when u is very small. However, it seems that it is nontrivial to evaluate ϵ_L and η_1 for the weak-coupling case; more precise estimates on $\sin^2 k_j$'s should be necessary when u is very small.

For the case when (B.5) is valid, the quantity ϵ_L should be very small if the following inequality holds:

$$\left|p^{-1}\frac{\alpha}{2-\alpha}\right| < 1. \tag{B.8}$$

For the region: $p_{c2} < p < p_{c3}$ $(1 < \alpha < 2)$, however, the inequality (B.8) does not hold for all values of α satisfying $1 < \alpha < 2$. Let us consider the case of $u \gg 1$. When u is very large, we can approximate $1/p$ by $1/(2\alpha u)$ using the relation: $p = \alpha u + \sqrt{1+\alpha^2 u^2}$. Then we can show that the inequality (B.8) holds under the following condition:

$$\alpha < 2 - \frac{1}{2u}. \tag{B.9}$$

Thus, at least for the case of $u \gg 1$, we have shown that the boundary solutions k_L and v_1 are stable when $1 < \alpha < 2 - 1/(2u)$, where $2 - 1/(2u)$ is very close to the critical point $\alpha = 2$. For the region: $p > p_{c3}$ $(\alpha > 2)$, we can show, under the condition $u \gg 1$, that the boundary solutions k_L and v_1 are stable if $\alpha > 2 + 1/(2u)$.

Similarly, we can discuss the case when the evaluation (B.6) is valid, where there are the three boundary solutions, k_L, k_1 and v_1. For the strong-coupling case, we can explicitly show that the boundary solutions are stable if $\alpha > 2 + 1/(2u)$; we have the following:

$$p^{-1}|z_1|^{-1}\frac{\alpha}{\alpha-2} < 1 \qquad \text{when } \alpha > 2 + 1/(2u). \tag{B.10}$$

Let us now consider the boundary solutions for the case when $p < 0$.

$$\begin{aligned} k_1' &= \mathrm{i}\kappa - \mathrm{i}\delta_1' \qquad \text{for } 0 < \alpha < 1 \\ v_1' &= \mathrm{i}(\alpha-1)u + \mathrm{i}\eta_1' \qquad \text{for } 1 < \alpha < 2 \\ k_2' &= \mathrm{i}\log\left((\alpha-2)u + \sqrt{(\alpha-2)^2u^2+1}\right) + \mathrm{i}\delta_2' \qquad \text{for } 2 < \alpha. \end{aligned} \tag{B.11}$$

Here δ_1', δ_2' and η_1' should be very small. We recall that for the case of $p < 0$, the boundary solutions k_1', k_2' and v_1' have been discussed in [15, 16]. For some convenience, we use symbols ϵ_1' and ϵ_2' defined in the following:

$$\sin k_1' = \mathrm{i}(\alpha-1)u + \mathrm{i}\epsilon_1' \qquad \sin k_L' = \mathrm{i}(\alpha-1)u + \epsilon_2' \tag{B.12}$$

which are related to δ_1' and δ_2' by

$$\epsilon_1' = -\cosh\kappa \times \delta_1' \qquad \epsilon_2' = \sqrt{(\alpha-2)^2u^2+1} \times \delta_2'.$$

Applying the formula (B.1), we can evaluate ϵ_1', η_1' and ϵ_2' as follows.

(1) When there is only one boundary solution k_1', we have

$$\epsilon_1' = \mathrm{O}(p^{-2L}). \tag{B.13}$$

(2) When there are two boundary solutions k_1' and v_1' and when $u > 1$, we have

$$\begin{aligned} |\epsilon_1' - \eta_1'| &= \mathrm{O}\left(\left(\frac{\alpha}{2-\alpha}\right)^{-2N}\right) \\ |\epsilon_1'| &= \mathrm{O}\left(\left(\frac{\alpha}{2-\alpha}\right)^{-2N} p^{-2L}\right). \end{aligned} \tag{B.14}$$

(3) When there are three boundary solutions k_1', k_2' and v_1' and when $u > 1$, we have

$$\begin{aligned} |\epsilon_2' - \eta_1'| &= \mathrm{O}(|z_2'|^{2L}) \\ |\epsilon_1' - \eta_1'| &= \mathrm{O}\left(|z_2'|^{2L}\left(\frac{\alpha}{\alpha-2}\right)^{-2N}\right) \\ |\epsilon_1'| &= \mathrm{O}\left(|z_2'|^{2L}\left(\frac{\alpha}{\alpha-2}\right)^{-2N} p^{-2L}\right). \end{aligned} \tag{B.15}$$

Here z_2' is given by

$$z_2' = \exp(\mathrm{i}k_2') = -(\alpha-2)u + \sqrt{(\alpha-2)^2u^2+1}.$$

We note that $|z_2| < 1$ when $\alpha > 2$.

We note that evaluations (B.13)–(B.15) can be applied for the ground-state solutions in the regions of $-p_{c2} < p < -p_{c1}$ $(0 < \alpha < 1)$, $-p_{c3} < p < -p_{c2}$ $(1 < \alpha < 2)$, and $p < -p_{c3}$ $(2 < \alpha)$. We also note that in the derivations of (B.14) and (B.15) we have made the same approximation as in (B.7).

When evaluations (B.13)–(B.15) are valid, the stability conditions for the boundary roots are satisfied for any p and u. When $p < -1$ and $u > 0$

$$|p|^{-1} < 1 \qquad \left|p^{-1}\frac{\alpha}{\alpha-2}\right| < 1 \qquad \left|p^{-1}z_2'\frac{\alpha}{\alpha-2}\right| < 1 \qquad \text{etc.} \quad \text{(B.16)}$$

However, we should remark that it is not certain whether (B.14) and (B.15) are valid also for the weak-coupling case: $u \ll 1$.

We now discuss how the boundary solutions of the open-boundary Hubbard model can be related to those of the interacting spin-$\frac{1}{2}$ fermion systems. We consider the case when the bandwidth $4t$ is very large and the electron density N/L is very small.

In order to show explicitly the effect of the large bandwidth, we replace u and p in equations (2), (4) and (5) by u/t and p/t, respectively. We recall that so far the energy scale has been normalized such that $t = 1$. Under the limit of $t \to \infty$, the critical points p_c's become the following:

$$\begin{aligned} &p_{c1}/t \to 1 \\ &p_{c2}/t \to 1 + u/t \\ &p_{c3}/t \to 1 + 2u/t. \end{aligned} \quad \text{(B.17)}$$

The values obtained in the limit are equivalent to the critical points of the boundary parameter [17] for the interacting spin-$\frac{1}{2}$ fermions.

When the electron density N/L is very small, the Fermi wavenumber k_F should be very small. Therefore, we can make linear approximations for the charge rapidities such as $\exp(\mathrm{i}k) \approx 1 + \mathrm{i}k$ and $\sin k \approx k$. Then, we can show that the boundary term in the Bethe ansatz equations of the open-boundary Hubbard model corresponds to that of the interacting spin-$\frac{1}{2}$ fermion system under the linear approximations

$$\frac{2k}{2\pi} - \frac{1}{2\pi\mathrm{i}}\ln\left(\frac{1+\exp(\mathrm{i}k)p/t}{1+\exp(-\mathrm{i}k)p/t}\right) \to -\frac{2}{2\pi}\tan^{-1}\left(\frac{k}{-(1+p/t)}\right). \quad \text{(B.18)}$$

Hereafter we may renormalize the boundary chemical potential p so that we can replace p/t by p. Thus, we have explicitly shown that when $t \gg 1$ and $N/L \ll 1$, the Bethe ansatz equations of the open-boundary 1D Hubbard model are reduced into those of the interacting spin-$\frac{1}{2}$ fermion system [17] with the open-boundary condition.

Under the large bandwidth and small electron-density limit, the boundary solutions of the open-boundary Hubbard model for the case of $p < 0$ remain intact. We can make the same approximation with (B.7), since $\sin^2 k_j$'s are very small. Here we note that the case of large bandwidth corresponds to the weak-coupling case where the approximation (B.7) may not be effective. When the density is very low, however, it is valid for some cases. For example, we may consider the case where N is fixed and L is proportional to t under the limit $t \to \infty$ so that each momentum k_j is proportional to $1/t$. Then, we can apply the approximation (B.7) for this case. In this way, the boundary solutions of the open Hubbard model for the case $p < 0$ are related to those of the interacting spin-$\frac{1}{2}$ fermion system discussed in [17].

For the case when $p > 0$, however, the boundary solutions of the open Hubbard model are not related to any solution of the interacting spin-$\frac{1}{2}$ fermion system. They exist only when the band is half-filled. The physical condition is completely different from the low-density case.

Appendix C. Particle–hole transformation for the open-boundary Hubbard chain

Let us denote by $d_{j,\sigma}$ and $d^{\dagger}_{j,\sigma}$, the annihilation and creation operators for the hole with spin σ on the jth site, respectively. We define a particle–hole transformation as follows. We replace the creation (annihilation) operator of electron with spin σ on the jth site by the annihilation (creation) operator of hole with spin σ on the jth site for $\sigma = \uparrow, \downarrow$ and for $j = 1, \ldots, L$, and then multiplying by the gauge factor $(-1)^j$ the hole operators on the jth site for all the sites:

$$c^{\dagger}_{j,\sigma} \to (-1)^j d_{j,\sigma} \qquad c_{j,\sigma} \to (-1)^j d^{\dagger}_{j,\sigma}. \tag{C.1}$$

The ground-state energy for $p > 0$ is related to that of $p < 0$ by the particle–hole transformation; the sign of the boundary chemical potential is changed under the transformation. Let us denote by $E(N_{\downarrow}, N_{\uparrow}; U, p)$ the ground-state energy for $N_{\downarrow}$ down-spin electrons, $N_{\uparrow}$ up-spin electrons with the Hubbard coupling U and the boundary chemical potential p. Then, applying the particle–hole transformation, we have the following:

$$E(L - M, L - M'; U, p) = E(M, M'; U, -p) + (L - N)U + 2p. \tag{C.2}$$

For the half-filled band, the ground-state energies for $p > 0$ and $p < 0$ are explicitly related. Recall we assume L is even. Then, we have the following:

$$E(L/2, L/2; U, p) = E(L/2, L/2; U, -p) + 2p. \tag{C.3}$$

On the other hand, it seems quite difficult to find out an explicit relation between the sets of the charge (spin) rapidities for the cases $p > 0$ and $p < 0$. It seems as though there might be a simple connection such as that for any momentum k in the ground state of $p > 0$ the value $\pi \pm k$ corresponds to one of the ground-state solutions for $p < 0$. However, this is not the case. There is no such relation between the boundary solutions k'_1, k'_2 and v'_1 for $p < -p_{c3}$ and the boundary solutions k_1, k_L and v_1 for $p > p_{c3}$.

Some numerical solutions of the Bethe ansatz equations suggest that it can be quite nontrivial to find any explicit relations between the sets of the half-filled ground-state solutions for the cases $p > 0$ and $p < 0$. Details should be discussed in future papers.

Appendix D. Boundary solutions for some excited states

We discuss the quantum numbers of some excited states with the boundary solutions. We assume the adiabatic hypothesis for the quantum numbers.

Let us consider an excited state which has only real-valued momenta and rapidities when $p = 0$. We denote by Δ^c_0 (Δ^s_0) the set of the quantum numbers for the momenta (rapidities). Let us denote by $\Delta^c(\Delta^s)$ the set of the quantum numbers of real-valued momenta in the excited state at a given value of p. In general, $\Delta^c(\Delta^s)$ depends on p. For the excited state we write by $\Delta^c_{\rm im}$ ($\Delta^s_{\rm im}$) the set of the quantum numbers of complex-valued momenta (rapidities). It is useful to introduce the notation for holes; we denote by $\Delta^c_{\rm hole}$ ($\Delta^s_{\rm hole}$) the set of the quantum numbers of holes for the real-valued momenta (rapidities). Then, we can define $Z^c_L(k)$, $Z^s_L(v)$, $z^c_B(k)$, and $z^s_B(v)$ also for the excited state; in the formulae (4) we replace Δ^c_g and Δ^s_g by Δ^c and Δ^s, respectively. Similarly to the ground state, we can evaluate the $I_{\rm min}$'s for the excited state as follows:

$$\begin{aligned} &I_{\rm min} = z^c_B(0) + 1 \qquad I_{\rm max} = L + z^c_B(\pi) - 1 \\ &J_{\rm min} = z^s_B(0) + 1 \\ &J_{\rm max} = (N - N_{\rm im}) - (M - M_{\rm im}) + (z^s_B(\infty) - \tfrac{1}{2}). \end{aligned} \tag{D.1}$$

Here $N_{\rm im}$ and $M_{\rm im}$ denote the number of complex-valued charge and spin rapidities (boundary solutions), respectively. We recall that N and M denote the number of electrons and that of down-spins, respectively.

For an illustration, let us discuss the boundary solutions of an excited state for the case when $p < 0$. Hereafter we assume $N < L$. We consider the excited state of N electrons with M down-spins where the quantum number at $p = 0$ is given by the following:

$$\begin{aligned} &\Delta_0^c = \{1, 3, 4, \ldots, N+1\} \qquad \Delta_0^s = \{1, 2, \ldots, M\} \\ &\Delta_{\rm im}^c = \Delta_{\rm im}^s = \phi. \end{aligned} \tag{D.2}$$

It follows from (D.1) that when $p = 0$ the sets of holes are given by

$$\Delta_{\rm hole}^c = \{2, N+2, N+3, \ldots, L\} \qquad \Delta_{\rm hole}^s = \{M+1, \ldots, N-M\}. \tag{D.3}$$

Here we note that when $L = N + 1$, then we have $\Delta_{\rm hole}^c = \{2\}$, and also that when N is even and $M = N/2$, then we have $\Delta_{\rm hole}^s = \phi$. Applying the formulae (10) and (D.1), we can show that there are four critical points given by $-p_{cj}$ for $j = 1, \ldots, 4$. We have the following five cases when $p < 0$.

(1) For $-p_{c1} < p < 0$, we have no boundary solution. We have a hole at $I = 2$.

$$\begin{aligned} &\Delta_{\rm im}^c = \Delta_{\rm im}^s = \phi \\ &\Delta^c = \{1, 3, 4, \ldots, N+1\} \qquad \Delta^s = \{1, 2, \ldots, M\} \\ &\Delta_{\rm hole}^c = \{2, N+2, \ldots, L\} \qquad \Delta_{\rm hole}^s = \{M+1, \ldots, N-M\}. \end{aligned}$$

(2) For $-p_{c2} < p < -p_{c1}$, we have k_1' and a hole at $I = 2$.

$$\begin{aligned} &\Delta_{\rm im}^c = \{1\} \qquad \Delta_{\rm im}^s = \phi \\ &\Delta^c = \{3, 4, \ldots, N+1\} \qquad \Delta^s = \{1, 2, \ldots, M\} \\ &\Delta_{\rm hole}^c = \{2, N+2, \ldots, L\} \qquad \Delta_{\rm hole}^s = \{M+1, \ldots, N-M\}. \end{aligned}$$

(3) For $-p_{c3} < p < -p_{c2}$, we have k_1' and v_1' and a hole at $I = 2$.

$$\begin{aligned} &\Delta_{\rm im}^c = \{1\} \qquad \Delta_{\rm im}^s = \{1\} \\ &\Delta^c = \{3, 4, \ldots, N+1\} \qquad \Delta^s = \{2, 3, \ldots, M\} \\ &\Delta_{\rm hole}^c = \{2, N+2, \ldots, L\} \qquad \Delta_{\rm hole}^s = \{M+1, \ldots, N-M\}. \end{aligned}$$

(4) For $-p_{c4} < p < -p_{c3}$, we have k_1' and v_1' but no hole at $I = 2$. A new hole appears at $I = L + 1$.

$$\begin{aligned} &\Delta_{\rm im}^c = \{1\} \qquad \Delta_{\rm im}^s = \{1\} \\ &\Delta^c = \{3, 4, \ldots, N+1\} \qquad \Delta^s = \{2, 3, \ldots, M\} \\ &\Delta_{\rm hole}^c = \{N+2, \ldots, L+1\} \qquad \Delta_{\rm hole}^s = \{M+1, \ldots, N-M\}. \end{aligned}$$

(5) For $p < -p_{c4}$, we have k_1' and v_1'. A new hole appears at $J = 1$.

$$\begin{aligned} &\Delta_{\rm im}^c = \{1\} \qquad \Delta_{\rm im}^s = \{1\} \\ &\Delta^c = \{3, 4, \ldots, N+1\} \qquad \Delta^s = \{2, 3, \ldots, M\} \\ &\Delta_{\rm hole}^c = \{N+2, \ldots, L+1\} \qquad \Delta_{\rm hole}^s = \{1, M+1, \ldots, N-M\}. \end{aligned}$$

We recall $p_{c4} = 3u + \sqrt{1 + (3u)^2}$.

Let us consider the ground state and the excited state discussed in the last paragraph. For the two regions $-p_{c4} < p < -p_{c3}$ and $p < -p_{c4}$, the ground-state solutions have the same structure, while the excited state solutions have different structures; the excited state has two boundary solutions k_1 and v_1 for both of the regions, however, it has a different numbers of holes in the spin rapidities for each of the two regions. Thus, it is suggested that there can be more subtle points in the boundary excitations than had been described in [17]

for those of the interacting spin-$\frac{1}{2}$ fermion system. However, it seems that some physical interpretations similar to those in [17] should be valid also for the boundary excitations of the open-boundary Hubbard model. Some precise investigations should be discussed in later publications.

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