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Wave function in the strong coupling limit of the Hubbard open chain

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Abstract. The one-dimensional repulsive Hubbard model with infinitely strong interactions is studied under the open boundary condition. The ground-state wave function of the present model is derived based on the Bethe *ansatz* method. Using the wave functions thus obtained, the Friedel oscillations in the Hubbard open chain are discussed.

1. Introduction

Recently, effects of nonmagnetic impurities in low-dimensional quantum systems have attracted much attention, see e.g. [1]. In a one-dimensional magnet, such as the Heisenberg chain, a nonmagnetic impurity cuts the magnetic chain. Therefore, in such purely one-dimensional systems, we may often recognize the effects of nonmagnetic impurities as those of boundaries. In general, the presence of an impurity or a boundary in uniform systems yields oscillations in densities, which are called the Friedel oscillations. Using numerical methods, the Friedel oscillations have been studied in some one-dimensional models, e.g. the spinless fermion model [2], the Kondo lattice model [3], the Hubbard model [4] etc. The asymptotic behaviour of the oscillations has been also discussed using the bosonization technique [5, 6], and the Bethe *ansatz* method [7, 4], based on the boundary conformal field theory. However, few results on the Friedel oscillations have been directly derived from the wave function, although the Bethe *ansatz* wave functions were obtained for several one-dimensional quantum systems with boundaries, e.g. the Heisenberg model [8–10], the Hubbard model [11–14] and so on.

In the present paper, we study the wave function in the large-u limit of the Hubbard model with boundaries based on the Bethe *ansatz* method. Using the wave function, we discuss the Friedel oscillations of the Hubbard open chain in the large-u limit.

In our discussions, we describe the Hubbard open chain by the following Hamiltonian,

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

where $p_{\pm}^{\mathrm{L}}$ (or $p_{\pm}^{\mathrm{R}}$) denotes the magnitude of the boundary field for the electron with spin $\pm$ on the left-end (or right-end) site. Here, the symbol $c_{j\sigma}$ (or $c_{j\sigma}^{\dagger}$) denotes the annihilation (or the creation) operator of an electron with spin σ at site j, and $n_{j\sigma}$ stands for the

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number operator of the electron. The symbol L denotes the number of sites. We consider the situation where $(N - M)$ electrons have up spins and M electrons have down spins $(L \geqslant N \geqslant M)$.

At first (in section 2), we take the limit $u \to +\infty$ in the Bethe *ansatz* wave function of the present model with free boundaries. Consequently, we observe that the ground-state wave function takes a simple form in this limit, owing to a decoupling of charge and spin degrees of freedom. Namely, in the large-u limit the charge sector is described as the wave function of the spinless fermion model with boundaries, while the spin sector is equivalent to the antiferromagnetic Heisenberg open chain. Under the periodic boundary condition, such a strong coupling limit was discussed by Ogata and Shiba [15] using the Lieb–Wu solution [16]. For recent investigations based on their analysis [15], see e.g. [17] and references cited therein.

Next, in section 3, we discuss the large-u limit of the Hubbard chain with boundary fields. Within an assumption, we also obtain a decoupling of charge and spin sectors for finite boundary fields.

In section 4, we discuss the Friedel oscillations in the large-u limit of the Hubbard open chain. For this purpose, we calculate the electron density and the magnetization as a functions of coordinates, using the factorized form of the wave function obtained in section 2.

In section 5, we summarize our results obtained with our discussions.

2. Bethe *ansatz* wave function in the strong coupling limit of the Hubbard open chain

In the present section, we derive the ground-state wave function of the Hubbard open chain with infinitely strong repulsive interactions. We mainly discuss the free boundary case in this section. Effects of the boundary fields are studied in the next section.

At first, as preliminaries, we have to recapitulate the Bethe *ansatz* analysis for an arbitrary u [11–14]. (See also [18].) For more detailed derivations of the Bethe *ansatz* equations, refer to the work by Shiroishi and Wadati [13]. In the present paper we use different notations from theirs [13] so that we can easily take the large-u limit.

We describe the amplitude in the wave function of the Hamiltonian (1.1) by the symbol $\psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N)$. Namely, the state vector $|\psi\rangle$ takes the following form,

$$|\psi\rangle = \sum_{\{(x_j,\sigma_j)\}} \psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N)|x_1\sigma_1,\ldots,x_N\sigma_N\rangle \tag{2.1}$$

with $|x_1\sigma_1,\ldots,x_N\sigma_N\rangle \equiv c^\dagger_{x_1\sigma_1}\ldots c^\dagger_{x_N\sigma_N}|0\rangle$, where we have no electrons in the vacuum $|0\rangle$. Under the extended Bethe *ansatz*, we describe the wave function by

$$\psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N) = \sum_P A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{P1},\ldots,k_{PN}) \exp\left(\mathrm{i}\sum_{j=1}^{N} k_{Pj}x_{Qj}\right) \tag{2.2}$$

in the region $1 \leqslant x_{Q1} \leqslant \cdots \leqslant x_{QN} \leqslant L$, where Q means a permutation of N coordinates. The summation $\sum_P$ in (2.2) runs over all permutations and negations of $(k_1,\ldots,k_N)$. We substitute ψ, equation (2.2), into the eigenvalue equation $\mathcal{H}|\psi\rangle = E|\psi\rangle$ to obtain the following relationships:

$$\begin{aligned} &A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{P1},\ldots,k_{Pn+1}=j,k_{Pn}=i,\ldots,k_{PN}) \\ &\quad = \frac{(\sin k_i - \sin k_j)P_{nn+1} - \mathrm{i}2u}{(\sin k_i - \sin k_j) + \mathrm{i}2u} A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{P1},\ldots,k_{Pn}=i,k_{Pn+1} \\ &\quad = j,\ldots,k_{PN}) \end{aligned} \tag{2.3}$$

$$A_{\sigma_{Q1},\ldots}(-k_{P1},\ldots)=-\frac{1-p^{\mathrm{L}}_{\sigma_{Q1}}\,\mathrm{e}^{+\mathrm{i}k_{P1}}}{1-p^{\mathrm{L}}_{\sigma_{Q1}}\,\mathrm{e}^{-\mathrm{i}k_{P1}}}A_{\sigma_{Q1},\ldots}(k_{P1},\ldots) \tag{2.4}$$

$$A_{\ldots,\sigma_{QN}}(\ldots,-k_{PN})=-\mathrm{e}^{\mathrm{i}2(L+1)k_{PN}}\frac{1-p^{\mathrm{R}}_{\sigma_{QN}}\,\mathrm{e}^{-\mathrm{i}k_{PN}}}{1-p^{\mathrm{R}}_{\sigma_{QN}}\,\mathrm{e}^{+\mathrm{i}k_{PN}}}A_{\ldots,\sigma_{QN}}(\ldots,k_{PN}) \tag{2.5}$$

where P_{nn+1} is a permutation operator for the interchange between Qn and $Q(n+1)$. We remark that $p^{\mathrm{L}}_{\sigma_{Q1}}$ takes $p^{\mathrm{L}}_{\pm}$ for $\sigma_{Q1}=\pm$. Similarly, $p^{\mathrm{R}}_{\sigma_{QN}}$ takes $p^{\mathrm{R}}_{\pm}$ for $\sigma_{QN}=\pm$. The energy eigenvalue E is given by

$$E=-2\sum_{j=1}^{N}\cos k_j. \tag{2.6}$$

We can derive all the coefficients $\{A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{P1},\ldots,k_{PN})\}_P$ from $A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_1,\ldots,k_N)$ with $\mathrm{Re}(k_j)>0$, using the above relationships. The coefficient $A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_1,\ldots,k_N)$ takes the form:

$$A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_1,\ldots,k_N)=\varepsilon_Q\times\phi \tag{2.7}$$

where the symbol ε_Q denotes the sign of the permutation Q, and ϕ is a component of the vector $\boldsymbol{\phi}$ given by the eigenvalue equation:

$$T_j\boldsymbol{\phi}=\boldsymbol{\phi} \tag{2.8}$$

$$\begin{aligned}T_j\equiv{}&S_{j,j-1}(k_j,k_{j-1})\ldots S_{j,1}(k_j,k_1)s(k_j;\,p^{\mathrm{L}}_{\sigma_j})S_{1,j}(k_1,-k_j)\ldots S_{j-1,j}(k_{j-1},-k_j)\\&\times S_{j+1,j}(k_{j+1},-k_j)\ldots S_{N,j}(k_N,-k_j)s(k_j;\,p^{\mathrm{R}}_{\sigma_j})\\&\times S_{j,N}(k_j,k_N)\ldots S_{j,j+1}(k_j,k_{j+1})\,\mathrm{e}^{\mathrm{i}2(L+1)k_j}\end{aligned} \tag{2.9}$$

$$S_{i,j}(k_i,k_j)\equiv\frac{\sin k_i-\sin k_j+\mathrm{i}2uP_{ij}}{\sin k_{\mathrm{i}}-\sin k_j+\mathrm{i}2u}\qquad s(k_j;\,p_{\sigma_i})\equiv\frac{1-p_{\sigma_i}\mathrm{e}^{-\mathrm{i}k_j}}{1-p_{\sigma_i}e^{+\mathrm{i}k_j}}. \tag{2.10}$$

Then the eigenvector $\boldsymbol{\phi}$ has ${}_NC_M$ components, each of which is characterized by spin coordinates, i.e. the locations of M down spins $\{y_\beta\}$ ($\beta=1,\ldots,M$). In equation (2.10), P_{ij} stands for the permutation operator which acts on the spin coordinates.

Indeed, we can diagonalize T_j for the four cases in table 1 [13, 14] by taking the following form of ϕ:

$$\begin{aligned}\phi(y_1,\ldots,y_M)\equiv{}&\sum_P B(\lambda_{P1},\ldots,\lambda_{PM})\\&\times\prod_{\beta=1}^{M}\left[(\sin k_1+\lambda_{P\beta}-\mathrm{i}u)\prod_{j=1}^{y_\beta-1}\frac{\sin k_j-\lambda_{P\beta}+\mathrm{i}u}{\sin k_{j+1}-\lambda_{P\beta}-\mathrm{i}u}\right]\end{aligned} \tag{2.11}$$

with $1\leqslant y_1\leqslant\cdots\leqslant y_M\leqslant N$. The summation $\sum_P$ in (2.11) runs over all permutations and negations of $(\lambda_1,\ldots,\lambda_N)$. Except for a constant factor, the coefficient $B(\lambda_{P1},\ldots,\lambda_{PM})$ can take the following form

$$\begin{aligned}B(\lambda_{P1},\ldots,\lambda_{PM})=\varepsilon_P\prod_{\alpha=1}^{M}&\left[\mathcal{B}(\lambda_{P\alpha})\prod_{j=1}^{N}\left(\frac{\lambda_{P\alpha}-\sin k_j+\mathrm{i}u}{\lambda_{P\alpha}-\sin k_j-\mathrm{i}u}\frac{\lambda_{P\alpha}+\sin k_j+\mathrm{i}u}{\lambda_{P\alpha}+\sin k_j-\mathrm{i}u}\right)^{1/2}\right]\\&\times\prod_{1\leqslant\alpha<\beta\leqslant M}(\lambda_{P\alpha}-\lambda_{P\beta}-\mathrm{i}2u)(\lambda_{P\alpha}+\lambda_{P\beta}-\mathrm{i}2u)\end{aligned} \tag{2.12}$$

with

$$\prod_{j=1}^{N}\frac{\lambda_\alpha-\sin k_j+\mathrm{i}u}{\lambda_\alpha-\sin k_j-\mathrm{i}u}\frac{\lambda_\alpha+\sin k_j+\mathrm{i}u}{\lambda_\alpha+\sin k_j-\mathrm{i}u}=Y(\lambda_\alpha)\prod_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M}\frac{\lambda_\alpha-\lambda_\beta+\mathrm{i}2u}{\lambda_\alpha-\lambda_\beta-\mathrm{i}2u}\frac{\lambda_\alpha+\lambda_\beta+\mathrm{i}2u}{\lambda_\alpha+\lambda_\beta-\mathrm{i}2u} \tag{2.13}$$

for $\alpha = 1, \ldots, M$, where ε_P is a sign factor which changes the sign at each of the permutations and negations. In the above equations, we have used the symbols $\mathcal{B}$ and Y defined by

$$\mathcal{B}(\lambda) \equiv \begin{cases} 1 \text{ for cases A and C} \\ \eta^{-\frac{1}{2}}(\lambda;\, p^{\mathrm{R}}) \text{ for cases B and D} \end{cases} \qquad \eta(\lambda;\, p) \equiv \frac{\mathrm{i}(\frac{1}{2}(p^{-1} - p) + u) + \lambda}{\mathrm{i}(\frac{1}{2}(p^{-1} - p) + u) - \lambda} \tag{2.14}$$

$$Y(\lambda) \equiv \begin{cases} 1 \text{ for case A} & \eta(\lambda;\, p^{\mathrm{L}})\eta(\lambda;\, p^{\mathrm{R}}) \text{ for case B} \\ \eta(\lambda;\, p^{\mathrm{L}}) \text{ for case C} & \eta(\lambda;\, p^{\mathrm{R}}) \text{ for case D.} \end{cases} \tag{2.15}$$

We can also obtain the eigenvalue of T_j. The eigenvalue equation (2.8) means that the eigenvalue is equal to unity, so that we have

$$\mathrm{e}^{\mathrm{i}2(L+1)k_j} Z(k_j) = \prod_{\beta=1}^{M} \frac{\sin k_j - \lambda_\beta + \mathrm{i}u}{\sin k_j - \lambda_\beta - \mathrm{i}u} \frac{\sin k_j + \lambda_\beta + \mathrm{i}u}{\sin k_j + \lambda_\beta - \mathrm{i}u} \tag{2.16}$$

for $j = 1, \ldots, N$, where

$$Z(k_j) \equiv \zeta(k_j;\, p^{\mathrm{L}})\zeta(k_j;\, p^{\mathrm{R}}) \qquad \zeta(k;\, p) \equiv \frac{1 - p\,\mathrm{e}^{-\mathrm{i}k}}{1 - p\,\mathrm{e}^{+\mathrm{i}k}}. \tag{2.17}$$

Then, we have two kinds of condition, equations (2.16) and (2.13) among the numbers $\{k_j\}$ $(j = 1, \ldots, N)$ and $\{\lambda_\alpha\}$ $(\alpha = 1, \ldots, M)$, which are the Bethe *ansatz* equations of the present model (1.1).

Now, we take the limit $u \to \infty$ and derive the ground-state wave function. In the remaining part of the present section, we discuss the free boundary case (i.e. $p_\pm^{\mathrm{L}} = p_\pm^{\mathrm{R}} = 0$), for simplicity. Namely, we have $Z(k_j) = 1$, $Y(\lambda_\alpha) = 1$ and $\mathcal{B}(\lambda_\alpha) = 1$. The cases with finite boundary fields are treated in the next section.

We introduce the new rapidities $\{\Lambda_\alpha\}$ by $\Lambda_\alpha = \lambda_\alpha/(2u)$, to scale $\{\lambda_\alpha\}$ by u. We assume that each of the rapidities $\{k_j\}$ $(j = 1, \ldots, N)$ and $\{\Lambda_\alpha\}$ $(\alpha = 1, \ldots, M)$ corresponding to the ground state is of order u^0 for $u \sim \infty$.

Under this assumption, at first, we consider the strong coupling limit of the wave function. We remark that the matrix connecting two coefficients in equation (2.3) goes to -1 in this limit. Moreover, we combine equations (2.4), (2.5), (2.7) and (2.9) to arrive at a factorized form of the wave function;

$$\psi = \psi_{\mathrm{c}}(x_{Q1}, \ldots, x_{QN}) \times \phi_{\mathrm{s}}(y_1, \ldots, y_M) + \mathrm{O}\left(\frac{1}{u}\right) \tag{2.18}$$

$$\psi_{\mathrm{c}}(x_{Q1}, \ldots, x_{QN}) = \varepsilon_Q \sum_P a_P \exp\left(\mathrm{i} \sum_{j=1}^{N} k_{Pj} x_{Qj}\right) \tag{2.19}$$

$$\phi_{\mathrm{s}}(y_1, \ldots, y_M) = \sum_P b_P \prod_{\alpha=1}^{M} \left(\frac{\Lambda_{P\alpha} - \frac{\mathrm{i}}{2}}{\Lambda_{P\alpha} + \frac{\mathrm{i}}{2}}\right)^{y_\alpha - \frac{1}{2}} \tag{2.20}$$

except for a constant factor. Here, the summations in equations (2.19) and (2.20) run over all permutations and negations in $(k_1, \ldots, k_N)$ and $(\Lambda_1, \ldots, \Lambda_M)$, respectively. The coefficients a_P and b_P take the following forms:

$$a_P = \varepsilon_P \qquad b_P = \varepsilon_P \prod_{\alpha=1}^{M} \left(\frac{\Lambda_{P\alpha} + \frac{\mathrm{i}}{2}}{\Lambda_{P\alpha} - \frac{\mathrm{i}}{2}}\right)^N \times \prod_{1 \leqslant \alpha < \beta \leqslant M} (\Lambda_{P\alpha} - \Lambda_{P\beta} - \mathrm{i})(\Lambda_{P\alpha} + \Lambda_{P\beta} - \mathrm{i}) \tag{2.21}$$

where each symbol ε_P denotes the sign factor which changes the sign at each mutation of P. We remark that we can rewrite ψ_c as

$$\psi_c(x_{Q1}, \ldots, x_{QN}) = (2i)^N \varepsilon_Q \det(\sin k_i x_{Qj}). \tag{2.22}$$

Next, we take the large-u limit in the Bethe *ansatz* equations (2.16) and (2.13) to have

$$1 = e^{i2(L+1)k_j} \qquad \left(\frac{\Lambda_\alpha + \frac{i}{2}}{\Lambda_\alpha - \frac{i}{2}}\right)^{2N} = \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{\Lambda_\alpha - \Lambda_\beta + i}{\Lambda_\alpha - \Lambda_\beta - i} \frac{\Lambda_\alpha + \Lambda_\beta + i}{\Lambda_\alpha + \Lambda_\beta - i}. \tag{2.23}$$

Taking the logarithm of each equation, we can obtain the following forms

$$2\pi I_j = 2(L+1)k_j \tag{2.24}$$

$$2\pi J_\alpha = (2N+1)\theta(2\Lambda_\alpha) - \sum_{\beta=1}^{M}\{\theta(\Lambda_\alpha - \Lambda_\beta) + \theta(\Lambda_\alpha + \Lambda_\beta)\} \tag{2.25}$$

with $\theta(x) \equiv 2\tan^{-1} x$, where $\{I_j\}$ and $\{J_\alpha\}$ take integer values. The ground state corresponds to

$$\{I_j\} = \{1, 2, \ldots, N-1, N\} \qquad \{J_\alpha\} = \{1, 2, \ldots, M-1, M\}. \tag{2.26}$$

Using the rapidities thus obtained, the energy eigenvalue (2.6) can be described as

$$E = -2\sum_{j=1}^{N} \cos k_j + \frac{2}{u(L+1)} \sum_{j=1}^{N} \sin^2 k_j \sum_{\alpha=1}^{M} \frac{-\frac{1}{2}}{\Lambda_\alpha^2 + \frac{1}{4}} + O\left(\frac{1}{u^2}\right). \tag{2.27}$$

Then, we find that ψ_c takes the form of the wave function for the spinless fermion model with boundaries and, on the other hand, ϕ_s takes the form of that for the antiferromagnetic Heisenberg model with boundaries. Refer to [8–10, 18].

3. Effects of boundary fields

In the present section, we derive the ground-state wave function of the Hubbard open chain with boundary fields. Instead of taking the same strategies as those in the previous section, we study the large-u limit by expanding the matrix T_j (2.9).

In our discussions, we recognize that boundary chemical potentials are of order u^0, while we parametrize boundary magnetic fields as $p^L = q^L/(2u)$ and $p^R = q^R/(2u)$ with $q^{L,R} \sim O(u^0)$. See table 1. For these boundary fields, we assume that $\{k_j\}$ and $\{\sin k_j\}$ $(j = 1, \ldots, N)$ are of order u^0 in the ground state.

If we have some complex $\sin k_j$ of order u^1 in the ground state, the energy (2.6) of the state can be of order u. This suggests that, in such a state, there exist electron pairs occupying the same sites. Therefore, our assumption may physically mean that the ground state of the present model, equation (1.1), at $u = \infty$ is given as a superposition of only the states in which all the electrons occupy different sites and have an energy of order u^0. (Of course, we expect that the ground state contains the doubly occupied states as the higher-order contributions of u^{-1} for $u \to \infty$.) The works by Bedürftig and Frahm [20] and Deguchi *et al* [21] support our assumption.

Under the above assumption, the matrix S_{ij} equation (2.10), can be expanded as follows,

$$S_{i,j}(k_i, k_j) = P_{ij} + \frac{\sin k_i - \sin k_j}{2ui}(1 - P_{ij}) + O\left(\frac{1}{u^2}\right). \tag{3.1}$$

Table 1. The Bethe *ansatz* equations of the Hubbard model (1.1) have been derived for the four kinds of boundary field [13, 14] shown in the second column. We call the boundary chemical potential 'type-a boundary field', and call the boundary magnetic field 'type-b boundary field'. In taking the large-u limit, we take the parametrization listed in the third column.

Cases	Boundary fields	For $u \to \infty$
Case A	$p_+^{\mathrm{L}} = p_-^{\mathrm{L}} \equiv p^{\mathrm{L}}$	$p^{\mathrm{L}} \sim \mathrm{O}(u^0)$
(type aa)	$p_+^{\mathrm{R}} = p_-^{\mathrm{R}} \equiv p^{\mathrm{R}}$	$p^{\mathrm{R}} \sim \mathrm{O}(u^0)$
Case B	$p_+^{\mathrm{L}} = -p_-^{\mathrm{L}} \equiv p^{\mathrm{L}}$	$p^{\mathrm{L}} \equiv q^{\mathrm{L}}/(2u) \sim \mathrm{O}(u^{-1})$
(type bb)	$p_+^{\mathrm{R}} = -p_-^{\mathrm{R}} \equiv p^{\mathrm{R}}$	$p^{\mathrm{R}} \equiv q^{\mathrm{R}}/(2u) \sim \mathrm{O}(u^{-1})$
Case C	$p_+^{\mathrm{L}} = -p_-^{\mathrm{L}} \equiv p^{\mathrm{L}}$	$p^{\mathrm{L}} \equiv q^{\mathrm{L}}/(2u) \sim \mathrm{O}(u^{-1})$
(type ba)	$p_+^{\mathrm{R}} = p_-^{\mathrm{R}} \equiv p^{\mathrm{R}}$	$p^{\mathrm{R}} \sim \mathrm{O}(u^0)$
Case D	$p_+^{\mathrm{L}} = p_-^{\mathrm{L}} \equiv p^{\mathrm{L}}$	$p^{\mathrm{L}} \sim \mathrm{O}(u^0)$
(type ab)	$p_+^{\mathrm{R}} = -p_-^{\mathrm{R}} \equiv p^{\mathrm{R}}$	$p^{\mathrm{R}} \equiv q^{\mathrm{R}}/(2u) \sim \mathrm{O}(u^{-1})$

Using this form, we arrive at the following results:

$$T_j = \mathrm{e}^{\mathrm{i}2(L+1)k_j}\mathcal{Z}(k_j)\left\{\mathcal{I} - \frac{2\mathrm{i}\sin k_j}{u}\mathcal{H}_{\mathrm{s}}\right\} + \mathrm{O}\left(\frac{1}{u^2}\right) \tag{3.2}$$

with

$$\mathcal{Z}(k_j) = \begin{cases} \dfrac{1-p^{\mathrm{L}}\,\mathrm{e}^{-\mathrm{i}k_j}}{1-p^{\mathrm{L}}\,\mathrm{e}^{+\mathrm{i}k_j}}\dfrac{1-p^{\mathrm{R}}\,\mathrm{e}^{-\mathrm{i}k_j}}{1-p^{\mathrm{R}}\,\mathrm{e}^{+\mathrm{i}k_j}} \text{ for case A} & 1 \text{ for case B} \\ \dfrac{1-p^{\mathrm{R}}\,\mathrm{e}^{-\mathrm{i}k_j}}{1-p^{\mathrm{R}}\,\mathrm{e}^{+\mathrm{i}k_j}} \text{ for case C} & \dfrac{1-p^{\mathrm{L}}\,\mathrm{e}^{-\mathrm{i}k_j}}{1-p^{\mathrm{L}}\,\mathrm{e}^{+\mathrm{i}k_j}} \text{ for case D} \end{cases} \tag{3.3}$$

where $\mathcal{I}$ denotes the identity operator and $\mathcal{H}_{\mathrm{s}}$ stands for the Hamiltonian of the antiferromagnetic Heisenberg open chain defined by

$$\mathcal{H}_{\mathrm{s}} \equiv \begin{cases} \mathcal{H}_{\mathrm{s}}^{(0)} \text{ for case A} & \mathcal{H}_{\mathrm{s}}^{(0)} - \dfrac{q^{\mathrm{L}}}{2}\sigma_1^z - \dfrac{q^{\mathrm{R}}}{2}\sigma_N^z \text{ for case B} \\ \mathcal{H}_{\mathrm{s}}^{(0)} - \dfrac{q^{\mathrm{L}}}{2}\sigma_1^z \text{ for case C} & \mathcal{H}_{\mathrm{s}}^{(0)} - \dfrac{q^{\mathrm{R}}}{2}\sigma_N^z \text{ for case D} \end{cases} \tag{3.4}$$

$$\mathcal{H}_{\mathrm{s}}^{(0)} \equiv \sum_{j=1}^{N-1}\frac{1}{2}(P_{jj+1}-1) = \sum_{j=1}^{N-1}\left(\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1} - \frac{1}{4}\right). \tag{3.5}$$

As we have discussed in the previous section, we have to diagonalize T_j, see (2.8). If we neglect the terms of order u^{-2}, we can take the eigenfunction of the Heisenberg model with boundary fields as that of the matrix T_j (3.2). Then, the eigenvalue t_j of the matrix T_j is given by

$$t_j = \mathrm{e}^{\mathrm{i}2(L+1)k_j}\mathcal{Z}(k_j)\left\{\mathcal{I} - \frac{2\mathrm{i}\sin k_j}{u}E_{\mathrm{s}}(\{\lambda_\alpha\})\right\} + \mathrm{O}\left(\frac{1}{u^2}\right) \tag{3.6}$$

with

$$E_{\mathrm{s}}(\{\lambda_\alpha\}) \equiv \begin{cases} E_{\mathrm{s}}^{(0)}(\{\lambda_\alpha\}) \text{ for case A} & E_{\mathrm{s}}^{(0)}(\{\lambda_\alpha\}) - \dfrac{q^{\mathrm{L}}}{2} - \dfrac{q^{\mathrm{R}}}{2} \text{ for case B} \\ E_{\mathrm{s}}^{(0)}(\{\lambda_\alpha\}) - \dfrac{q^{\mathrm{L}}}{2} \text{ for case C} & E_{\mathrm{s}}^{(0)}(\{\lambda_\alpha\}) - \dfrac{q^{\mathrm{R}}}{2} \text{ for case D} \end{cases} \tag{3.7}$$

$$E_{\mathrm{s}}^{(0)}(\{\lambda_\alpha\}) \equiv \sum_{\alpha=1}^{M}\frac{-\frac{1}{2}}{\Lambda_\alpha^2 + \frac{1}{4}}. \tag{3.8}$$

Here, $\{\Lambda_\alpha\}$ ($\alpha = 1, \ldots, M$) satisfy the Bethe *ansatz* equation of the Heisenberg open chain with boundary fields [9, 10], namely

$$\left(\frac{\Lambda_\alpha + \frac{\mathrm{i}}{2}}{\Lambda_\alpha - \frac{\mathrm{i}}{2}}\right)^{2N} = \mathcal{Y}(\Lambda_\alpha) \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{\Lambda_\alpha - \Lambda_\beta + \mathrm{i}}{\Lambda_\alpha - \Lambda_\beta - \mathrm{i}} \frac{\Lambda_\alpha + \Lambda_\beta + \mathrm{i}}{\Lambda_\alpha + \Lambda_\beta - \mathrm{i}} \tag{3.9}$$

with

$$\mathcal{Y}(\Lambda_\alpha) = \begin{cases} 1 \text{ for case A} \\ \dfrac{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{L}}}+1)+\Lambda_\alpha}{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{L}}}+1)-\Lambda_\alpha} \dfrac{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{R}}}+1)+\Lambda_\alpha}{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{R}}}+1)-\Lambda_\alpha} \text{ for case B} \\ \dfrac{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{L}}}+1)+\Lambda_\alpha}{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{L}}}+1)-\Lambda_\alpha} \text{ for case C} \\ \dfrac{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{R}}}+1)+\Lambda_\alpha}{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{R}}}+1)-\Lambda_\alpha} \text{ for case D.} \end{cases} \tag{3.10}$$

The eigenvalue equation (2.8) means the condition $t_j = 1$ so that we have

$$1 = \mathrm{e}^{\mathrm{i}2(L+1)k_j} \mathcal{Z}(k_j) \tag{3.11}$$

neglecting higher order terms of u^{-1}. Using the parameters $\{k_j\}$ ($j = 1, \ldots, N$), $\{\lambda_\alpha\}$ ($\alpha = 1, \ldots, M$) determined by equations (3.11) and (3.9) we describe the energy eigenvalue as follows,

$$E = -2\sum_{j=1}^{N} \cos k_j + \frac{2E_{\mathrm{s}}(\{\lambda_\alpha\})}{u(L+1)} \sum_{j=1}^{N} \sin^2 k_j + \mathrm{O}\left(\frac{1}{u^2}\right). \tag{3.12}$$

By minimizing E, we can obtain the ground-state rapidities $\{k_j\}$ and $\{\lambda_\alpha\}$. Here, we have to remember that u is an arbitrary large number. Therefore, we can obtain $\{k_j\}$ by minimizing $-2\sum_j^N \cos k_j$ while, independently of this procedure, we can determine $\{\lambda_\alpha\}$ by minimizing E_{s}.

We find that the wave function takes the same form as that in the free-boundary case, i.e. (2.18) with (2.19), (2.20). However, the definitions of the coefficients a_P and b_P have to be changed as follows:

$$a_P = \varepsilon_P \prod_{j=1}^{N} [\mathcal{A}(k_{Pj})\, \mathrm{e}^{-\mathrm{i}(L+1)k_{Pj}}] \tag{3.13}$$

$$b_P = \varepsilon_P \prod_{\alpha=1}^{M} \left[\mathcal{B}(\Lambda_{P\alpha})\left(\frac{\Lambda_{P\alpha} + \frac{\mathrm{i}}{2}}{\Lambda_{P\alpha} - \frac{\mathrm{i}}{2}}\right)^{N}\right] \times \prod_{1\leqslant\alpha<\beta\leqslant M} (\Lambda_{P\alpha} - \Lambda_{P\beta} - \mathrm{i})(\Lambda_{P\alpha} + \Lambda_{P\beta} - \mathrm{i}) \tag{3.14}$$

with

$$\mathcal{A}(k_j) = \left(\frac{1 - p^{\mathrm{R}}\,\mathrm{e}^{+\mathrm{i}k_j}}{1 - p^{\mathrm{R}}\,\mathrm{e}^{-\mathrm{i}k_j}}\right)^{\frac{1}{2}} \qquad \mathcal{B}(\Lambda_\alpha) = 1 \text{ for cases A and C} \tag{3.15}$$

$$\mathcal{A}(k_j) = 1 \qquad \mathcal{B}(\Lambda_\alpha) = \left(\frac{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{R}}}+1)-\Lambda_\alpha}{\frac{\mathrm{i}}{2}(\frac{1}{q^{\mathrm{R}}}+1)+\Lambda_\alpha}\right)^{\frac{1}{2}} \text{ for cases B and D.} \tag{3.16}$$

Similarly to the free boundary case, the wave function is given as a product of two functions. One of them is the wave function of the spinless fermion model with boundary fields and the other is that of the antiferromagnetic Heisenberg model with boundary fields.

Table 2. The wave function in the large-u limit of the Hubbard open chain with boundary fields realizes a decoupling of charge and spin degrees of freedom. Namely, in this limit, the charge sector is described as the wave function of the spinless fermion model (SLF) with boundary fields, while the spin sector is equivalent to the antiferromagnetic Heisenberg model (AHM) with boundary fields. The boundary fields in the resulting models are listed.

	Boundary fields of SLF model		Boundary fields of AFH model	
Cases	Left	Right	Left	Right
Case A	p^{L}	p^{R}	0 (free)	0 (free)
Case B	0 (free)	0 (free)	q^{L}	q^{R}
Case C	0 (free)	p^{R}	q^{L}	0 (free)
Case D	p^{L}	0 (free)	0 (free)	q^{R}

See [8–10, 19]. The boundary fields in the resulting models are summarized in table 2. We remark that we can also derive the results obtained in this section by the method of the previous section.

4. Friedel oscillations of the Hubbard open chain in the strong coupling limit

In the present section, we study the Friedel oscillations of the Hubbard open chain in the strong coupling limit. Using the wave function obtained by our discussions, we calculate the ground-state averages of the electron number $\langle n_j \rangle$ and of the magnetization $\langle S_j^z \rangle$, where $n_j \equiv n_{j+} + n_{j-}$ and $S_j^z \equiv (n_{j+} - n_{j-})/2$.

The averages are given by the following forms:

$$\langle n_j \rangle = \frac{\sum_{1 \leqslant x_1 < \cdots < x_N \leqslant L} (\sum_{i=1}^{N} \delta_{x_i,j}) \times W_{\mathrm{c}}(x_1, \ldots, x_N)}{\sum_{1 \leqslant x_1 < \cdots < x_N \leqslant L} W_{\mathrm{c}}(x_1, \ldots, x_N)} \tag{4.1}$$

$$\langle S_j^z \rangle = \frac{\sum_{1 \leqslant x_1 < \cdots < x_N \leqslant L} (\sum_{i=1}^{N} m_i \delta_{x_i,j}) \times W_{\mathrm{c}}(x_1, \ldots, x_N)}{\sum_{1 \leqslant x_1 < \cdots < x_N \leqslant L} W_{\mathrm{c}}(x_1, \ldots, x_N)} \tag{4.2}$$

$$m_i = \frac{1}{2} - \frac{\sum_{1 \leqslant y_1 < \cdots < y_M \leqslant N} (\sum_{k=1}^{M} \delta_{y_k,i}) \times W_{\mathrm{s}}(y_1, \ldots, y_M)}{\sum_{1 \leqslant y_1 < \cdots < y_M \leqslant N} W_{\mathrm{s}}(y_1, \ldots, y_M)} \tag{4.3}$$

with

$$W_{\mathrm{c}}(x_1, \ldots, x_N) = \psi_{\mathrm{c}}^*(x_1, \ldots, x_N) \times \psi_{\mathrm{c}}(x_1, \ldots, x_N) \tag{4.4}$$

$$W_{\mathrm{s}}(y_1, \ldots, y_M) = \phi_{\mathrm{s}}^*(y_1, \ldots, y_M) \times \phi_{\mathrm{s}}(y_1, \ldots, y_M). \tag{4.5}$$

Here, ψ_{c} and ϕ_{s} have been defined in sections 2 and 3. We remark that we have the explicit form of $\langle n_j \rangle$ as follows,

$$\langle n_j \rangle = \frac{1}{L+1} \left\{ N + \frac{1}{2} \left(1 - \frac{\sin(\pi j/L + 1)(2N+1)}{\sin(\pi j/L + 1)} \right) \right\}. \tag{4.6}$$

For simplicity, we discuss only the free boundary case. Moreover, we focus on the states (1) near half-filling ($N = L - 1$ and $M = (L/2) - 1$) and (2) near quarter-filling ($N = (L/2) - 1$ and $M = (L/4) - 1$). At half-filling ($N = L$ and $M = L/2$), we have $\langle n_j \rangle = 1$ and $\langle S_j^z \rangle = 0$ for any j, because of the particle–hole symmetry and the spin up–down symmetry. At quarter-filling ($N = L/2$ and $M = L/4$) with $u \to \infty$, the particle–hole symmetry of the spinless fermion model and the up–down symmetry of the

Heisenberg model yield a uniform state with $\langle n_j \rangle = 1/2$ and $\langle S_j^z \rangle = 0$ for any j. However, in each case, $\langle n_j \rangle$ and $\langle S_j^z \rangle$ may oscillate by introducing one holon and one spinon due to the existence of the boundaries.

In general, the presence of impurities or boundaries in a one-dimensional system leads to Friedel oscillations in densities, which have the general form [4, 22, 23]

$$\delta\rho(x) \sim cx \frac{\cos(2k_{\mathrm{F}}x + \varphi)}{x^{\gamma}} + c'x \frac{\cos(4k_{\mathrm{F}}x + \varphi')}{x^{\gamma'}} \tag{4.7}$$

where k_{F} denotes the Fermi wave number of the free electron. For example, we have $k_{\mathrm{F}} = (\pi/2)$ (or $k_{\mathrm{F}} = (\pi/4)$) for the half filling (or the quarter-filling).

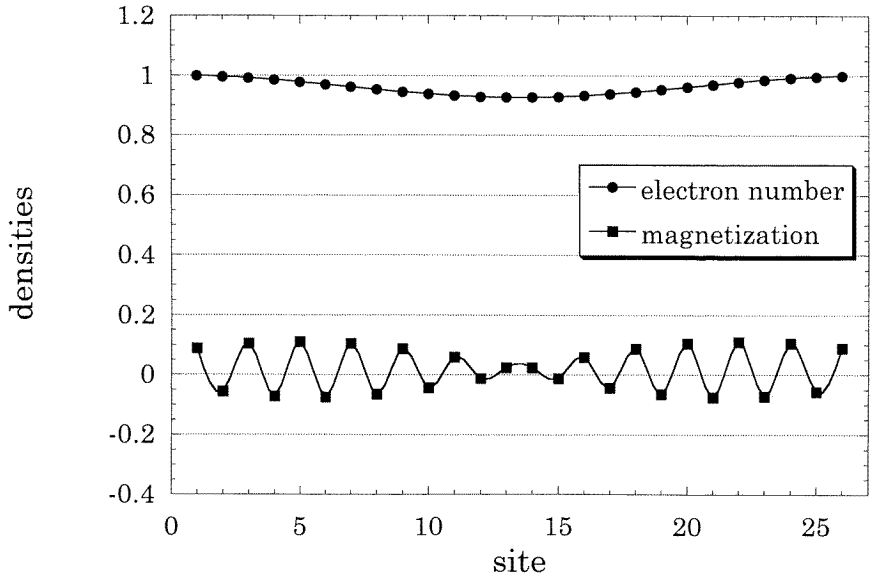

Figure 1. Oscillations of densities $\langle n_j \rangle$ and $\langle S_j^z \rangle$ on the 26-site Hubbard open chain near half-filling. We have taken the parameters $L = 26$, $N = 25$ and $M = 12$. In evaluating the densities, we have numerically diagonalized the antiferromagnetic Heisenberg open chain with 25 sites to derive the ground-state eigenfunction with total $S^z = \frac{1}{2}$. Curves are guides to the eye.

In figures 1 and 2, we show the result obtained by our scheme. We have numerically evaluated $\langle n_j \rangle$ and $\langle S_j^z \rangle$ using equations (4.1) and (4.2). We have no oscillations in electron densities or oscillations in magnetizations with the period of 2 sites, near half-filling. On the other hand, near quarter-filling, electron densities oscillate with the period of 2 sites and magnetizations oscillate with the period of 4 sites. Although our results may include many finite size effects, we can really obtain the oscillations expected from the general form (4.7).

In this calculation, we have derived ϕ_{s} by numerical diagonalization of the Heisenberg model, instead of using the Bethe *ansatz* wave-function form. The Bethe *ansatz* form of ϕ_{s} is given as a sum of M terms, each of which we have to evaluate after solving the Bethe *ansatz* equation. As the system size becomes larger, it rapidly gets difficult to calculate by using the Bethe *ansatz* form. In order to evaluate the wave function ϕ_{s} with higher accuracy and within shorter computing time, we had better diagonalize the Heisenberg Hamiltonian numerically. The similar strategy has been taken in [15].

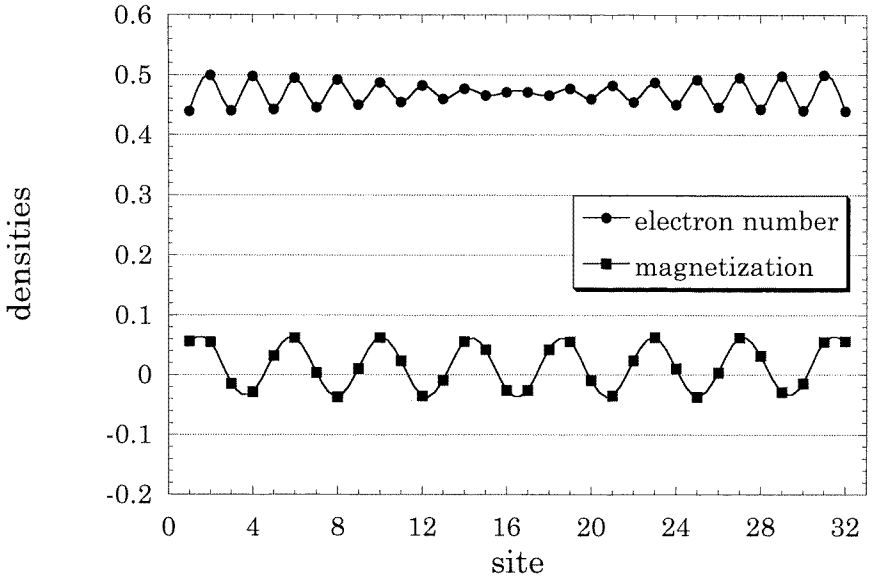

Figure 2. Oscillations of densities $\langle n_j \rangle$ and $\langle S_j^z \rangle$ on the 32-site Hubbard open chain near quarter-filling. We have taken the parameters $L = 32$, $N = 15$ and $M = 7$. In evaluating the densities, we have numerically diagonalized the antiferromagnetic Heisenberg open chain with 15 sites to derive the ground-state eigenfunction with total $S^z = \frac{1}{2}$. Curves are guides to the eye.

5. Summary

In the present paper, we have studied the strong coupling limit of the Hubbard open chain (1.1) based on the Bethe *ansatz* method.

In section 2, we have taken the strong coupling limit in the Bethe *ansatz* wave function of the present model (1.1) with free boundaries, so that we have obtained the product form of two functions, i.e. $\psi_c \times \phi_s$, as the ground-state wave function. Here, ψ_c denotes the wave function of the spinless fermion model and ϕ_s is that of the antiferromagnetic Heisenberg model. The boundary conditions of both resulting models are open.

Moreover, we have also derived the large-u limit wave function of the Hubbard open chain (1.1) with finite boundary fields, in section 3. Under an assumption, we have arrived at a similar form to the free boundary case. In this case, the resulting models, i.e. the spinless fermion model and the antiferromagnetic Heisenberg model, have also finite boundary fields.

In section 4, we have calculated the local electron number $\langle n_j \rangle$ and the local magnetization $\langle S_j^z \rangle$ in the Hubbard open chain with free boundaries, using the factorized form of the wave function obtained in section 2. Consequently we have obtained the Friedel oscillations in both quantities. In our results, the period of the oscillations in $\langle n_j \rangle$ (or $\langle S_j^z \rangle$) reflects the Fermi wave number in the charge (or the spin) sector, as is expected.

We can use the wave functions obtained in the present paper to evaluate various quantities in the Hubbard open chain with $u \to \infty$. We will report such results derived from the wave function elsewhere in the near future.

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