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Finite-size corrections in the XXZ model and the Hubbard model with boundary fields

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Abstract. The XXZ model and the Hubbard model with boundary fields are discussed. Using the exact solutions of the present models, the finite-size corrections of the ground-state energy and the low-lying excitation energies are calculated. The partition functions are also evaluated in the scaling limit. Through this calculation, the conformal weights of the primary fields in the present model are obtained.

1. Introduction

Recently, by using the finite-size scaling technique [1–3] based on conformal field theory [4], critical properties of one-dimensional quantum systems have been investigated, see for example [5–7]. In almost all of these investigations, one-dimensional systems under the periodic boundary condition are focused. On the other hand, in recent years, various integrable models on an open chain with boundary terms have been studied by the Bethe ansatz [8–11].

In the present paper, we discuss quantum systems on a chain with boundary fields, by using the finite-size scaling technique based on boundary conformal field theory (CFT) [12]. According to the boundary CFT, the partition function of a quantum critical system on the open chain with L sites is described as [13]

$$Z \equiv \mathrm{Tr}\, \mathrm{e}^{-\hat{H}/T} = \sum_h \mathcal{N}_h \chi_h \tag{1.1}$$

where $\hat{H}$ is the Hamiltonian of the relevant system, from which we subtract the terms of order L and L^0. The symbol $\mathcal{N}_h$ takes a non-negative integer, which depends on the boundary state. The symbol χ_h denotes the character of the highest-weight irreducible representation of the Virasoro algebra. We describe the conformal weight of the corresponding primary field by h. The character takes the following form:

$$\chi_h = q^{-c/24+h} \sum_{N=0}^{\infty} d_h(N) q^N \tag{1.2}$$

where the symbol c denotes the central charge. We describe the degeneracy of the states at the Nth level as $d_h(N)$. The above relation holds in the scaling limit $q \sim 0$, precisely. Therefore, by evaluating the partition function in the scaling limit, we can recognize the operator contents of the relevant model, namely which primary fields exist in the present model.

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In our previous paper [14], we discussed the operator contents of the XY model with a uniform magnetic field and a boundary field. We found that the XY model with a boundary field gives a representation of the shifted $U(1)$ Kac–Moody algebra [15]. In the previous work, we not only evaluated the partition function but also constructed the generators of the algebra by the operators in the XY model.

In the present paper, we discuss the operator contents of the XXZ model and the Hubbard model with boundary fields. Through this discussion, we find that each sector of these models also gives a representation of the algebra.

In section 2, we briefly review the exact solution of the XXZ model with a boundary field. The present model has been solved by Alcaraz *et al* [16] and Sklyanin [8]. In section 3, we derive the exact solution of the Hubbard model with a boundary field. In section 4, we evaluate the finite-size corrections for the energy of the present XXZ model. This calculation has been partially performed by Hamer and co-workers [17, 18]. In this sense, part of the contents of section 4 is a rederivation of their result, though our scheme is different from theirs. In section 5, we evaluate the finite-size corrections for the energy of the present Hubbard model. Using the result obtained in sections 4 and 5, we calculate the partition functions of the models in section 6. Through the form of the partition functions thus obtained, we discuss operator contents of the models in section 7. We also evaluate the surface critical exponents of classical systems corresponding to the present quantum systems with boundary fields.

2. Exact solution of the XXZ model with a boundary field

In the present section, we briefly review the exact solution of the XXZ model with a boundary field.

In the present paper, we discuss the XXZ model with a boundary field described by the following Hamiltonian:

$$\mathcal{H} = -\tfrac{1}{2}\sum_{j=1}^{L-1}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z) - \tfrac{1}{2}p(\sigma_1^z + \sigma_L^z) + \tfrac{1}{2}\Delta(L-1) \tag{2.1}$$

where the symbol σ_j^α denotes the α-component of the Pauli matrices at site j. We describe the length of the chain by L, which is assumed to take an even integer. We introduce a parameter γ as follows,

$$\Delta = -\cos\gamma \qquad \gamma \in [0, \pi). \tag{2.2}$$

Alcaraz *et al* [16] solved this model by the coordinate Bethe ansatz. Sklyanin [8] also solved it by the algebraic Bethe ansatz. Alcaraz *et al* introduced the following Bethe ansatz wavefunction [16]:

$$\psi(x_1, \ldots, x_M) = \sum_P \varepsilon_P A(k_{P1}, \ldots, k_{PM}) \exp\left(\mathrm{i}\sum_{j=1}^{M} k_{Pj}x_{Qj}\right) \tag{2.3}$$

where

$$1 \leqslant x_{Q1} < \cdots < x_{QM} \leqslant L \tag{2.4}$$

where the sum extends over all permutations and negations of $k_1, \ldots, k_M$ and ε_P takes a sign factor (± 1) and changes its sign at each such ‘mutation’. Thus, they obtained the Bethe ansatz equation

$$2L\phi(\eta_j,\gamma/2) = 2\pi I_j - 2\phi(\eta_j,\Gamma) + \sum_{\substack{l=1\\(l\neq j)}}^{M} (\phi(\eta_j-\eta_l,\gamma)+\phi(\eta_j+\eta_l,\gamma))$$
$$j = 1,\ldots,M \tag{2.5}$$

where

$$e^{2i\Gamma} = \frac{p-\Delta-e^{i\gamma}}{(p-\Delta)e^{i\gamma}-1} \qquad \phi(\eta,\gamma) = 2\tan^{-1}(\cot(\gamma)\tanh\eta). \tag{2.6}$$

Here, I_j takes a positive integer. The eigenenergy is given by

$$E = \sum_{j=1}^{M} 2(\Delta - \cos k_j) - p \qquad k_j = \phi(\eta_j,\gamma/2). \tag{2.7}$$

3. Exact solution of the Hubbard model with a boundary field

In the present section, we derive the exact solution of the Hubbard model with a boundary field.

We discuss the Hubbard model with a boundary field described by the following Hamiltonian:

$$\mathcal{H} = -\sum_{\sigma,j=1}^{L-1}(c_{j\sigma}^{\dagger}c_{j+1\sigma} + c_{j+1\sigma}^{\dagger}c_{j\sigma}) + U\sum_{j=1}^{L} n_{j+}n_{j-} + \mu\sum_{j=1}^{L}(n_{j+}+n_{j-})$$
$$-p_{+}(n_{1+}+n_{L+}) - p_{-}(n_{1-}+n_{L-}) \tag{3.1}$$

where the symbol $c_{j\sigma}$ ($c_{j\sigma}^{\dagger}$) denotes the annihilation (the creation) operator of an electron with spin σ at site j. The number operator of an electron is defined by $n_{j\sigma} \equiv c_{j\sigma}^{\dagger}c_{j\sigma}$. We describe the length of the chain by L, which is assumed to take an even integer. We discuss the present model with $U > 0$.

We assume the following wavefunction:

$$\psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N) = \sum_{P} \varepsilon_P A_{\sigma_{Q1},\ldots,\sigma_{QN}}(k_{PQ1},\ldots,k_{PQN}) \exp\left(i\sum_{j=1}^{N} k_{Pj}x_j\right) \tag{3.2}$$

where

$$1 \leqslant x_{Q1} \leqslant \cdots \leqslant x_{QN} \leqslant L. \tag{3.3}$$

The sum extends over all permutations and negations of $k_1,\ldots,k_N$ and ε_P takes a sign factor (± 1) and changes its sign at each such 'mutation'. We can evaluate scattering matrices as follows:

$$A_{\ldots\sigma_j,\sigma_i\ldots}(\ldots k_j,k_i\ldots) = S_{ij}(k_i,k_j)A_{\ldots\sigma_i,\sigma_j\ldots}(\ldots k_i,k_j\ldots) \tag{3.4}$$
$$A_{\sigma_i,\ldots}(-k_j,\ldots) = s^{L}(k_j;p_{\sigma_i})A_{\sigma_i,\ldots}(k_j,\ldots) \tag{3.5}$$
$$A_{\ldots,\sigma_i}(\ldots,-k_j) = s^{R}(k_j;p_{\sigma_i})A_{\ldots,\sigma_i}(\ldots,k_j) \tag{3.6}$$

where

$$S_{ij}(k_i,k_j) = \frac{\eta_i-\eta_j+i2uP_{ij}}{\eta_i-\eta_j+i2u} \tag{3.7}$$
$$s^{L}(k_j;p_\sigma) = (s(k_j;p_\sigma))^{-1} \qquad s^{R}(k_j;p_\sigma) = s(k_j;p_\sigma)e^{ik_j 2(L+1)} \tag{3.8}$$

with

$$\eta_j = \sin k_j \qquad u = \frac{U}{4} \qquad s(k_j; p_{\sigma_j}) = \frac{1 - p_{\sigma_j} e^{-ik_j}}{1 - p_{\sigma_j} e^{+ik_j}}. \tag{3.9}$$

Here, the operator P_{ij} interchanges the spin variables σ_i and σ_j. We note that using equations (3.4)–(3.6) we show that their 'mutant' relationships also hold, which are obtained from (3.4) by negations of $\{k_j\}$ and from (3.5) and (3.6) by permutations or negations of $\{k_j\}$.

By using these matrices, we obtain the following relationship:

$$A_{\ldots\sigma_j\ldots}(\ldots k_j \ldots) = T_j A_{\ldots\sigma_j\ldots}(\ldots k_j \ldots) \tag{3.10}$$

where

$$T_j = S_j^-(k_j) s(k_j; p_{\sigma_j}) R_j^-(k_j) R_j^+(k_j) s(k_j; p_{\sigma_j}) S_j^+(k_j) e^{ik_j 2(L+1)} \tag{3.11}$$

with

$$S_j^+(k_j) = S_{jN}(k_j, k_N) \times \cdots \times S_{jj+1}(k_j, k_{j+1}) \tag{3.12}$$

$$S_j^-(k_j) = S_{jj-1}(k_j, k_{j-1}) \times \cdots \times S_{j1}(k_j, k_1) \tag{3.13}$$

$$R_j^-(k_j) = S_{1j}(k_1, -k_j) \times \cdots \times S_{j-1j}(k_{j-1}, -k_j) \tag{3.14}$$

$$R_j^+(k_j) = S_{j+1j}(k_{j+1}, -k_j) \times \cdots \times S_{Nj}(k_N, -k_j). \tag{3.15}$$

Here, we define $S_j^- = R_j^- = I$ (the identity matrix) for $j = 1$ and $S_j^+ = R_j^+ = I$ for $j = L$. Therefore, we can obtain the (nested) Bethe ansatz equations by solving the following eigenvalue problem:

$$T_j \boldsymbol{t} = 1 \times \boldsymbol{t} \qquad j = 1, \ldots, N \tag{3.16}$$

where the symbol $\boldsymbol{t}$ denotes an eigenvector on the space of the spin variables. Detailed derivations from (3.2)–(3.16) are shown in the appendix. In the appendix, we give some examples of the Bethe ansatz wavefunctions for a few particles so that we can check the validity of the ansatz.

In the remaining part of the present paper, we restrict the boundary field to the following case:

$$p_\sigma = p \qquad \text{for } \sigma = \pm. \tag{3.17}$$

Then, since $s(k_j)$ does not depend on the spin variable, we only have to diagonalize the matrix $S_j^- R_j^- R_j^+ S_j^+$. This problem has been solved by Schulz [19] in the discussion on the free-boundary case, namely $p = 0$. We remark that this problem is also solved by the algebraic Bethe ansatz for an open chain [8]. Immediately, we can write the Bethe ansatz equations as follows:

$$e^{ik_j 2(L+1)} s^2(k_j; p) = \prod_{\beta=1}^{M} \frac{\eta_j - \lambda_\beta + iu}{\eta_j - \lambda_\beta - iu} \frac{\eta_j + \lambda_\beta + iu}{\eta_j + \lambda_\beta - iu} \tag{3.18}$$

$$\prod_{j=1}^{N} \frac{\lambda_\alpha - \eta_j + iu}{\lambda_\alpha - \eta_j - iu} \frac{\lambda_\alpha + \eta_j + iu}{\lambda_\alpha + \eta_j - iu} = \prod_{\substack{\beta=1 \\ (\beta\neq\alpha)}}^{M} \frac{\lambda_\alpha - \lambda_\beta + i2u}{\lambda_\alpha - \lambda_\beta - i2u} \frac{\lambda_\alpha + \lambda_\beta + i2u}{\lambda_\alpha + \lambda_\beta - i2u}$$

$$j = 1, \ldots, N \qquad \text{and} \qquad \alpha = 1, \ldots, M \tag{3.19}$$

where we assume that N takes an even integer. The eigenenergy is given by

$$E = \sum_{j=1}^{N} (\mu - 2\cos k_j). \tag{3.20}$$

We rewrite the present equations in the following form:

$$2Lk_j = 2\pi I_j - 2(k_j + \theta_0(k_j;\, p)) - \sum_{\beta=1}^{M}\left(2\tan^{-1}\frac{\eta_j - \lambda_\beta}{u} + 2\tan^{-1}\frac{\eta_j + \lambda_\beta}{u}\right) \tag{3.21}$$

$$\sum_{j=1}^{N}\left(2\tan^{-1}\frac{\lambda_\alpha - \eta_j}{u} + 2\tan^{-1}\frac{\lambda_\alpha + \eta_j}{u}\right)$$
$$= 2\pi J_\alpha + \sum_{\substack{\beta=1\\(\beta\neq\alpha)}}^{M}\left(2\tan^{-1}\frac{\lambda_\alpha - \lambda_\beta}{2u} + 2\tan^{-1}\frac{\lambda_\alpha + \lambda_\beta}{2u}\right)$$
$$j = 1, \ldots, N \qquad \text{and} \qquad \alpha = 1, \ldots, M \tag{3.22}$$

where

$$\theta_0(k;\, p) = \frac{1}{\mathrm{i}}\log s(k;\, p). \tag{3.23}$$

Here, I_j and J_α take integers.

4. Finite-size corrections of the XXZ model with a boundary field

In the present section, we evaluate the finite-size corrections for the spectrum of the present XXZ model (2.1), by using Woynarovich's scheme [5]. This calculation has been partially performed by Hamer and co-workers [17, 18]. In this sense, part of the contents of section 4 is a rederivation of their result, though our scheme is different from theirs. At the end of this section, we explain the relationship between their result and ours.

We rewrite the Bethe ansatz equation (2.5) for the present model as follows:

$$z_L(\eta_j) = \frac{I_j}{L} \qquad j = -M, \ldots, M \tag{4.1}$$

$$z_L(\eta) \equiv \frac{1}{\pi}\left\{p_0(\eta) + \frac{1}{L}q_0(\eta) - \frac{1}{2L}\sum_{j=-M}^{M}\phi(\eta - \eta_j, \gamma)\right\} \tag{4.2}$$

where

$$p_0(\eta) = \phi\left(\eta, \frac{\gamma}{2}\right) \qquad \text{and} \qquad q_0(\eta) = \phi(\eta, \Gamma) + \tfrac{1}{2}\phi(2\eta, \gamma) + \tfrac{1}{2}\phi(\eta, \gamma). \tag{4.3}$$

Here, we recognize η_{-j} as $-\eta_j$. When we describe the maximum and minimum values of $\{I_j\}$ as I^+ and I^-, respectively, we can introduce the integration boundaries Λ^+ and Λ^- by the following equations:

$$z_L(\Lambda^+) = \frac{1}{L}(I^+ + \tfrac{1}{2}) \qquad \text{and} \qquad z_L(\Lambda^-) = \frac{1}{L}(I^- - \tfrac{1}{2}). \tag{4.4}$$

In the present model, we find that the relationship $\Lambda^+ = -\Lambda^-$ ($I^+ = -I^-$) holds.

We define a density of roots $\{\eta_j\}$ as follows:

$$\sigma_L(\eta) \equiv \frac{\mathrm{d}}{\mathrm{d}\eta}z_L(\eta) \tag{4.5}$$

$$= \frac{1}{\pi}\left\{\frac{\mathrm{d}}{\mathrm{d}\eta}p_0(\eta) + \frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}\eta}q_0(\eta) - \frac{1}{2L}\sum_{j=-M}^{M}K(\eta - \eta_j)\right\} \tag{4.6}$$

where

$$K(\eta) \equiv \frac{\mathrm{d}}{\mathrm{d}\eta}\phi(\eta, \gamma). \tag{4.7}$$

Here, we introduce an integration operator $\boldsymbol{K}$ for a function $x(\eta)$ as follows:

$$\boldsymbol{K}_{\Lambda^+}(\eta|\eta')x(\eta') \equiv -\frac{1}{2\pi}\int_{-\Lambda^+}^{\Lambda^+} \mathrm{d}\eta'\, K(\eta-\eta')x(\eta'). \tag{4.8}$$

Moreover, we define an inner product for functions x and y by

$$(x, y) \equiv \tfrac{1}{2}\int_{-\Lambda^+}^{\Lambda^+} \mathrm{d}\eta'\, x(\eta')y(\eta'). \tag{4.9}$$

Then we find that the following relationship holds:

$$(y, \boldsymbol{K}x) = (\boldsymbol{K}y, x). \tag{4.10}$$

By using the Euler–Maclaurin formula, we can expand σ_L as

$$\sigma_L(\eta|\Lambda^+) = \sigma^{(0)}(\eta|\Lambda^+) + \frac{1}{L}\tau^{(0)}(\eta|\Lambda^+) - \frac{1}{24L^2}\frac{1}{\sigma_L(\Lambda^+|\Lambda^+)}\rho^{(0)}(\eta|\Lambda^+)$$
$$+\boldsymbol{K}_{\Lambda^+}(\eta|\eta')\sigma_L(\eta'|\Lambda^+) + o\left(\frac{1}{L^2}\right) \tag{4.11}$$

where

$$\sigma^{(0)}(\eta|\Lambda^+) = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\eta}p_0(\eta) \qquad \tau^{(0)}(\eta|\Lambda^+) = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\eta}q_0(\eta) \tag{4.12}$$

and

$$\rho^{(0)}(\eta|\Lambda^+) = \frac{1}{2\pi}(K'(\eta-\Lambda^+) - K'(\eta+\Lambda^+)). \tag{4.13}$$

Here, K' denotes a derivative of K. Moreover, we can obtain the following form:

$$\sigma_L(\eta|\Lambda^+) = \sigma(\eta|\Lambda^+) + \frac{1}{L}\tau(\eta|\Lambda^+) - \frac{1}{24L^2}\frac{\rho(\eta|\Lambda^+)}{\sigma_L(\Lambda^+|\Lambda^+)} + o\left(\frac{1}{L^2}\right) \tag{4.14}$$

where

$$\sigma(\eta|\Lambda^+) = \sigma^{(0)}(\eta|\Lambda^+) + \boldsymbol{K}_{\Lambda^+}(\eta|\eta')\sigma(\eta'|\Lambda^+) \tag{4.15}$$
$$\tau(\eta|\Lambda^+) = \tau^{(0)}(\eta|\Lambda^+) + \boldsymbol{K}_{\Lambda^+}(\eta|\eta')\tau(\eta'|\Lambda^+) \tag{4.16}$$

and

$$\rho(\eta|\Lambda^+) = \rho^{(0)}(\eta|\Lambda^+) + \boldsymbol{K}_{\Lambda^+}(\eta|\eta')\rho(\eta'|\Lambda^+). \tag{4.17}$$

We note that the formal solution of the following integration equation:

$$x(\eta|\Lambda^+) = x^{(0)}(\eta|\Lambda^+) + \boldsymbol{K}_{\Lambda^+}(\eta|\eta')x(\eta'|\Lambda^+) \tag{4.18}$$

is given as

$$x(\eta|\Lambda^+) = \sum_{n=0}^{\infty}\boldsymbol{K}^n_{\Lambda^+}(\eta|\eta')x^{(0)}(\eta'|\Lambda^+). \tag{4.19}$$

We can expand the energy spectrum (2.7) of the present model with respect to the powers of $1/L$, using the density of roots (4.14)

$$\frac{E}{L} = \frac{1}{L}\sum_{j=1}^{M}2(\Delta - \cos k_j) - \frac{p}{L} \tag{4.20}$$
$$= \varepsilon(\Lambda^+) + \frac{1}{L}\varphi(\Lambda^+) - \frac{1}{24L^2}\frac{e(\Lambda^+)}{\sigma_L(\Lambda^+|\Lambda^+)} + o\left(\frac{1}{L^2}\right) \tag{4.21}$$

where

$$\varepsilon(\Lambda^+) = (\varepsilon_d, \sigma^{(0)}) \tag{4.22}$$

$$\varphi(\Lambda^+) = (\varepsilon_d, \tau^{(0)}) - p - \tfrac{1}{2}\varepsilon_0(0) \tag{4.23}$$

and

$$e(\Lambda^+) = \frac{d}{d\Lambda^+}\varepsilon_0(\Lambda^+) + (\varepsilon_0, \rho) \tag{4.24}$$

with

$$\varepsilon_0(\eta) = 2(\Delta - \cos k) = \frac{-2\sin^2\gamma}{\cosh 2\eta - \cos\gamma} \tag{4.25}$$

and

$$\varepsilon_d(\eta|\Lambda^+) = \sum_{n=0}^{\infty} \boldsymbol{K}^n_{\Lambda^+}(\eta|\eta')\varepsilon_0(\eta'). \tag{4.26}$$

Here, we have used the relations $\Delta = -\cos\gamma$ and $\eta = \sin k$. The symbol ε_d denotes the dressed energy of the present model.

If the energy E is minimized for $\Lambda^+ = \Lambda$ in the thermodynamic limit, the parameter Λ is determined by

$$\frac{d}{d\Lambda^+}\varepsilon(\Lambda^+) = 0. \tag{4.27}$$

This equation is equivalent to

$$\varepsilon_d(\Lambda^+|\Lambda^+) = 0. \tag{4.28}$$

This relationship is the same as the corresponding condition in the periodic-boundary case. Therefore, we find that $\Lambda = \infty$. We remark that the relationship

$$\frac{d}{d\Lambda^+}\varphi_(\Lambda^+) = 0 \tag{4.29}$$

also holds for $\Lambda^+ = \Lambda$. Moreover, we find

$$\frac{d^2}{d\Lambda^{+2}}\varepsilon(\Lambda^+)\bigg|_{\Lambda^+=\Lambda} = e(\Lambda)\sigma(\Lambda|\Lambda). \tag{4.30}$$

Then, we obtain the following form as the expansion of the energy spectrum around the ground state:

$$E = L\varepsilon(\Lambda) + \varphi(\Lambda) + \frac{1}{L}\frac{e(\Lambda)}{\sigma_L(\Lambda|\Lambda)}(\tfrac{1}{2}L^2(\Lambda^+ - \Lambda)^2(\sigma(\Lambda|\Lambda))^2 - \tfrac{1}{24}) + o\left(\frac{1}{L^2}\right). \tag{4.31}$$

Taking

$$\int_{-\Lambda^+}^{\Lambda^+} \sigma_L(\eta)\, d\eta = \frac{2M+1}{L} \tag{4.32}$$

into account, we find that the following relationship holds for $\Lambda^+ - \Lambda$ infinitesimal:

$$(\Lambda^+ - \Lambda)\sigma(\Lambda|\Lambda)L = \frac{1}{\xi(\Lambda)}(\Delta M - \Theta(p)) \tag{4.33}$$

where

$$\Theta(p) \equiv \frac{\pi - \gamma - 2\Gamma}{2(\pi - \gamma)} = \frac{1}{2(\pi - \gamma)}\left\{\tan^{-1}\left(\frac{\tan\gamma}{1 - R(p)}\right) - \gamma\right\} \tag{4.34}$$

with

$$R(p) = \frac{2p}{\Delta(1-(p-\Delta)^2)}. \tag{4.35}$$

Here, the symbol ΔM denotes the deviation of M from its grand-state value, namely $L/2$, and takes an integer. The symbol ξ expresses the dressed charge, which is defined as

$$\xi(\eta) = \sum_{n=0}^{\infty} (\boldsymbol{K}_\Lambda)^n 1. \tag{4.36}$$

Since this definition is the same as that of the corresponding value in the periodic-boundary case, we know that it takes the following form [5]

$$\xi \equiv \xi(\Lambda) = \frac{1}{\sqrt{2(1-\gamma/\pi)}}. \tag{4.37}$$

Here, we evaluate the sound velocity of the present model v_s. Using the Bethe ansatz equation (2.5), we obtain the following relationship:

$$\sum_{j=-M}^{M} k_j = \pi \sum_{j=-M}^{M} \frac{I_j}{L}. \tag{4.38}$$

From this equation, we can recognize the dressed momentum $p_\mathrm{d}(\eta_j)$ as $\pi I_j/L$. Therefore, we can evaluate the sound velocity as follows:

$$v_\mathrm{s} = \left.\frac{\mathrm{d}\varepsilon_\mathrm{d}(\eta)}{\mathrm{d}p_\mathrm{d}(\eta)}\right|_{\eta=\Lambda} = \frac{e(\Lambda)}{\pi\sigma(\Lambda|\Lambda)}. \tag{4.39}$$

This quantity seems to be twice as large as the corresponding value in the periodic-boundary case [5]. However, this velocity is equal to that of the system with the periodic boundary condition, since this density of roots is twice as large as that of the periodic-boundary case [5]. In fact, we obtain the following form:

$$v_\mathrm{s} = \frac{\pi \sin\gamma}{\gamma}. \tag{4.40}$$

Summing up the above discussions, we can describe the energy spectrum around the ground state as follows:

$$E(\Delta M) = Le_\infty + f_\infty + \frac{\pi v_\mathrm{s}}{L}\left\{\frac{1}{2}\frac{(\Delta M - \Theta(p))^2}{\xi^2} - \frac{1}{24}\right\} + o\left(\frac{1}{L}\right) \tag{4.41}$$

where

$$e_\infty = \varepsilon(\Lambda) \qquad \text{and} \qquad f_\infty = \varphi(\Lambda). \tag{4.42}$$

We can express these quantities as follows:

$$e_\infty = \frac{1}{2}\int_{-\infty}^{+\infty} \mathrm{d}\lambda \, \frac{\sin^2\gamma}{\cosh 2\gamma\lambda - \cos\gamma} \frac{1}{\cosh \pi\lambda} \tag{4.43}$$

and

$$f_\infty = -p + \frac{\pi}{2}\frac{\sin\gamma}{\gamma} + \int_{-\infty}^{+\infty} \mathrm{d}\eta \, \varepsilon_0(\eta)(\tau_1(\eta) + \tau_2(\eta)) \tag{4.44}$$

with

$$\tau_1(\eta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega \, \frac{\sinh(\frac{1}{2}\omega\pi - \omega\Gamma)}{\sinh\frac{1}{2}\omega\pi + \sinh(\frac{1}{2}\omega\pi - \omega\gamma)} \mathrm{e}^{-\mathrm{i}\omega\eta} \tag{4.45}$$

$$\tau_2(\eta) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega \, \frac{\cosh\frac{1}{4}\omega\pi \, \sinh(\frac{1}{4}\omega\pi - \frac{1}{2}\omega\gamma)}{\sinh\frac{1}{2}\omega\pi + \sinh(\frac{1}{2}\omega\pi - \omega\gamma)} \mathrm{e}^{-\mathrm{i}\omega\eta}. \tag{4.46}$$

In order to obtain the complete form of the low-lying spectrum, we consider a particle–hole excitation in the vicinity of the Fermi surface. We describe a particle–hole pair

$$z_L(\eta_{\mathrm{p}}) = \frac{I_{\mathrm{p}}}{L} \qquad \text{and} \qquad z_L(\eta_{\mathrm{h}}) = \frac{I_{\mathrm{h}}}{L}. \tag{4.47}$$

By introducing the following half-odd numbers n_{p} and n_{h},

$$I_{\mathrm{p}} = I^+ + \tfrac{1}{2} + n_{\mathrm{p}} \qquad \text{and} \qquad I_{\mathrm{h}} = I^+ + \tfrac{1}{2} - n_{\mathrm{h}} \tag{4.48}$$

we characterize a particle–hole excitation by the positive integer

$$n_{\mathrm{ph}} \equiv n_{\mathrm{p}} + n_{\mathrm{h}}. \tag{4.49}$$

Since the presence of this particle–hole pair modifies σ_L by

$$\frac{\eta_{\mathrm{p}} - \eta_{\mathrm{h}}}{L} \rho(\eta|\Lambda^+) \tag{4.50}$$

this excitation changes the energy by

$$\frac{n_{\mathrm{ph}}}{L} \frac{e(\Lambda^+)}{\sigma_L(\Lambda^+)}. \tag{4.51}$$

If several pairs of particle and hole exist, we have to replace n_{ph} by N_+, where

$$N_+ = \sum_{\text{all pairs}} n_{\mathrm{ph}} \tag{4.52}$$

is a non-negative integer.

Finally, we obtain the energy spectrum around the ground state as follows:

$$E(\Delta M, N_+) = Le_\infty + f_\infty + \frac{\pi v_{\mathrm{s}}}{L} \left\{ \frac{1}{2} \frac{(\Delta M - \Theta(p))^2}{\xi^2} - \frac{1}{24} + N_+ \right\} + o\left(\frac{1}{L}\right). \tag{4.53}$$

Here, ΔM takes integers and N_+ takes non-negative integers. For a given N_+, the degeneracy is given by Euler's partition number $P(N_+)$. Hamer and co-workers [17, 18] evaluated finite-size corrections of the ground-state energy for a given ΔM. Our result $E(\Delta M, 0)$ coincides with theirs.

5. Finite-size corrections of the Hubbard model with a boundary field

In the present section, we evaluate the finite-size corrections for the spectrum of the present Hubbard model (3.1), by using Woynarovich's scheme [6].

We rewrite the Bethe ansatz equations (3.21) and (3.22) for the present model as follows:

$$z_L^{\mathrm{c}}(k_j) = \frac{I_j}{L} \qquad \text{and} \qquad z_L^{\mathrm{s}}(\lambda_\alpha) = \frac{J_\alpha}{L}$$
$$j = -N, \ldots, N \qquad \text{and} \qquad \alpha = -M, \ldots, M \tag{5.1}$$

$$z_L^{\mathrm{c}}(k) \equiv \frac{1}{\pi} \left\{ k + \frac{1}{L} p_0(k) + \frac{1}{2L} \sum_{\beta=-M}^{M} 2 \tan^{-1}\left(\frac{\sin k - \lambda_\beta}{u} \right) \right\} \tag{5.2}$$

$$z_L^{\mathrm{s}}(\lambda) \equiv \frac{1}{\pi} \left\{ \frac{1}{L} q_0(\lambda) + \frac{1}{2L} \sum_{j=-N}^{N} 2 \tan^{-1}\left(\frac{\lambda - \sin k_j}{u} \right) - \frac{1}{2L} \sum_{\beta=-M}^{M} 2 \tan^{-1}\left(\frac{\lambda - \lambda_\beta}{2u} \right) \right\} \tag{5.3}$$

where $u = U/4$ and

$$p_0(k) = k - \tan^{-1}\left(\frac{\sin k}{u} \right) + \theta_0(k; p) \qquad \text{and} \qquad q_0(\lambda) = \tan^{-1}\left(\frac{\lambda}{2u} \right). \tag{5.4}$$

Here, we recognize k_{-j} as $-k_j$ and $\lambda_{-\alpha}$ as $-\lambda_\alpha$. When we describe the maximum and minimum values of $\{I_j\}$ ($\{J_\alpha\}$) as I^+ and I^- (J^+ and J^-), respectively, we can introduce the integration boundaries k^+ and k^- (λ^+ and λ^-) by the following equations:

$$z_L^{\mathrm{c}}(k^+) = \frac{1}{L}(I^+ + \tfrac{1}{2}) \qquad \text{and} \qquad z_L^{\mathrm{c}}(k^-) = \frac{1}{L}(I^- - \tfrac{1}{2}) \tag{5.5}$$

and

$$z_L^{\mathrm{s}}(\lambda^+) = \frac{1}{L}(J^+ + \tfrac{1}{2}) \qquad \text{and} \qquad z_L^{\mathrm{s}}(\lambda^-) = \frac{1}{L}(J^- - \tfrac{1}{2}). \tag{5.6}$$

In the present model, we find that relationships $k^+ = -k^-$ ($I^+ = -I^-$) and $\lambda^+ = -\lambda^-$ ($J^+ = -J^-$) hold.

We define the densities of roots $\{k_j\}$ and $\{\lambda_\alpha\}$ as follows:

$$\sigma_L^{\mathrm{c}}(k) \equiv \frac{\mathrm{d}}{\mathrm{d}k} z_L^{\mathrm{c}}(k) \tag{5.7}$$

$$= \frac{1}{\pi}\left\{1 + \frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}k}p_0(k) + \frac{1}{2L}\sum_{\beta=-M}^{M} K_1(\sin k - \lambda_\beta)\cos k\right\} \tag{5.8}$$

and

$$\sigma_L^{\mathrm{s}}(\lambda) \equiv \frac{\mathrm{d}}{\mathrm{d}\lambda} z_L^{\mathrm{s}}(\lambda) \tag{5.9}$$

$$= \frac{1}{\pi}\left\{\frac{1}{L}\frac{\mathrm{d}}{\mathrm{d}\lambda}q_0(\lambda) + \frac{1}{2L}\sum_{j=-M}^{M} K_1(\lambda - \sin k_j) - \frac{1}{2L}\sum_{\beta=-N}^{N} K_2(\lambda - \lambda_\beta)\right\} \tag{5.10}$$

where

$$K_1(x) \equiv \frac{2u}{u^2 + x^2} \qquad \text{and} \qquad K_2(x) \equiv \frac{4u}{4u^2 + x^2}. \tag{5.11}$$

Here, we introduce an integration operator $\boldsymbol{K}$ for a two-component function $\boldsymbol{x} = (x^{\mathrm{c}}(k), x^{\mathrm{s}}(\lambda))^{\mathrm{T}}$ as follows:

$$\boldsymbol{K}_{k^+\lambda^+}(k, \lambda | k', \lambda')\boldsymbol{x}(k', \lambda') \tag{5.12}$$

$$\equiv \begin{pmatrix} \dfrac{\cos k}{2\pi}\displaystyle\int_{-\lambda^+}^{\lambda^+} \mathrm{d}\lambda'\, K_1(\sin k - \lambda')x^{\mathrm{s}}(\lambda') \\ \dfrac{1}{2\pi}\displaystyle\int_{-k^+}^{k^+} \mathrm{d}k'\, K_1(\lambda - \sin k')x^{\mathrm{c}}(k') - \dfrac{1}{2\pi}\displaystyle\int_{-\lambda^+}^{\lambda^+} \mathrm{d}\lambda'\, K_2(\lambda - \lambda')x^{\mathrm{s}}(\lambda') \end{pmatrix}. \tag{5.13}$$

Moreover, we define an inner product for two-component functions $\boldsymbol{x}$ and $\boldsymbol{y}$ by

$$(\boldsymbol{x}, \boldsymbol{y}) \equiv \tfrac{1}{2}\int_{-k^+}^{k^+} \mathrm{d}k'\, x^{\mathrm{c}}(k')y^{\mathrm{c}}(k') + \tfrac{1}{2}\int_{-\lambda^+}^{\lambda^+} \mathrm{d}\lambda'\, x^{\mathrm{s}}(\lambda')y^{\mathrm{s}}(\lambda'). \tag{5.14}$$

We define a transpose operator of $\boldsymbol{K}$ as

$$\boldsymbol{K}^{\mathrm{T}}_{k^+\lambda^+}(k, \lambda | k', \lambda')\boldsymbol{x}(k', \lambda')$$

$$\equiv \begin{pmatrix} \dfrac{1}{2\pi}\displaystyle\int_{-\lambda^+}^{\lambda^+} \mathrm{d}\lambda'\, K_1(\sin k - \lambda')x^{\mathrm{s}}(\lambda') \\ \dfrac{1}{2\pi}\displaystyle\int_{-k^+}^{k^+} \mathrm{d}k'\, \cos k' K_1(\lambda - \sin k')x^{\mathrm{c}}(k') - \dfrac{1}{2\pi}\displaystyle\int_{-\lambda^+}^{\lambda^+} \mathrm{d}\lambda'\, K_2(\lambda - \lambda')x^{\mathrm{s}}(\lambda') \end{pmatrix} \tag{5.15}$$

so that the following relationship holds:

$$(\boldsymbol{y}, \boldsymbol{K}\boldsymbol{x}) = (\boldsymbol{K}^{\mathrm{T}}\boldsymbol{y}, \boldsymbol{x}). \tag{5.16}$$

By using the Euler–Maclaurin formula, we can expand $\boldsymbol{\sigma}_L = (\sigma_L^{\mathrm{c}}, \sigma_L^{\mathrm{s}})^{\mathrm{T}}$ as

$$\begin{aligned}\boldsymbol{\sigma}_L(k, \lambda|k^+, \lambda^+) = {} & \boldsymbol{\sigma}^{(0)}(k, \lambda|k^+, \lambda^+) + \frac{1}{L}\boldsymbol{\tau}^{(0)}(k, \lambda|k^+, \lambda^+) \\ & + \frac{1}{24L^2}\frac{1}{\sigma_L^{\mathrm{c}}(k^+|k^+, \lambda^+)}\boldsymbol{\rho}_1^{(0)}(k, \lambda|k^+, \lambda^+) \\ & + \frac{1}{24L^2}\frac{1}{\sigma_L^{\mathrm{s}}(\lambda^+|k^+, \lambda^+)}\boldsymbol{\rho}_2^{(0)}(k, \lambda|k^+, \lambda^+) \\ & + \boldsymbol{K}_{k^+\lambda^+}(k, \lambda|k', \lambda')\boldsymbol{\sigma}_L(k', \lambda'|k^+, \lambda^+) + o\left(\frac{1}{L^2}\right)\end{aligned} \tag{5.17}$$

where

$$\boldsymbol{\sigma}^{(0)}(k, \lambda|k^+, \lambda^+) = \begin{pmatrix} \frac{1}{\pi} \\ 0 \end{pmatrix} \qquad \boldsymbol{\tau}^{(0)}(k, \lambda|k^+, \lambda^+) = \begin{pmatrix} \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}k}p_0(k) \\ \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\eta}q_0(\eta) \end{pmatrix} \tag{5.18}$$

and

$$\boldsymbol{\rho}_1^{(0)}(k, \lambda|k^+, \lambda^+) = \begin{pmatrix} 0 \\ \frac{\cos k^+}{2\pi}(K_1'(\lambda - \sin k^+) - K_1'(\lambda + \sin k^+)) \end{pmatrix} \tag{5.19}$$

$$\boldsymbol{\rho}_2^{(0)}(k, \lambda|k^+, \lambda^+) = \begin{pmatrix} \frac{\cos k}{2\pi}(K_1'(\sin k - \lambda^+) - K_1'(\sin k + \lambda^+)) \\ \frac{-1}{2\pi}(K_2'(\lambda - \lambda^+) - K_2'(\lambda + \lambda^+)) \end{pmatrix}. \tag{5.20}$$

Here, K_1' and K_2' denote derivatives of K_1 and K_2, respectively. Moreover, we can obtain the following form:

$$\begin{aligned}\boldsymbol{\sigma}_L(\eta|\Lambda^+) = {} & \boldsymbol{\sigma}(\eta|\Lambda^+) + \frac{1}{L}\boldsymbol{\tau}(\eta|\Lambda^+) + \frac{1}{24L^2}\frac{\boldsymbol{\rho}_1(k, \lambda|k^+, \lambda^+)}{\sigma_L^{\mathrm{c}}(k^+, \lambda^+|k^+, \lambda^+)} \\ & + \frac{1}{24L^2}\frac{\boldsymbol{\rho}_2(k, \lambda|k^+, \lambda^+)}{\sigma_L^{\mathrm{s}}(k^+, \lambda^+|k^+, \lambda^+)} + o\left(\frac{1}{L^2}\right)\end{aligned} \tag{5.21}$$

where

$$\boldsymbol{\sigma}(k, \lambda|k^+, \lambda^+) = \boldsymbol{\sigma}^{(0)}(k, \lambda|k^+, \lambda^+) + \boldsymbol{K}_{k^+\lambda^+}(k, \lambda|k', \lambda')\boldsymbol{\sigma}(k', \lambda'|k^+, \lambda^+) \tag{5.22}$$

$$\boldsymbol{\tau}(k, \lambda|k^+, \lambda^+) = \boldsymbol{\tau}^{(0)}(k, \lambda|k^+, \lambda^+) + \boldsymbol{K}_{k^+\lambda^+}(k, \lambda|k', \lambda')\boldsymbol{\tau}(k', \lambda'|k^+, \lambda^+) \tag{5.23}$$

and for $i = 1, 2$

$$\boldsymbol{\rho}_i(k, \lambda|k^+, \lambda^+) = \boldsymbol{\rho}_i^{(0)}(k, \lambda|k^+, \lambda^+) + \boldsymbol{K}_{k^+\lambda^+}(k, \lambda|k', \lambda')\boldsymbol{\rho}_i(k', \lambda'|k^+, \lambda^+). \tag{5.24}$$

We remark that the formal solution of the integration equation

$$\boldsymbol{x}(k, \lambda|k^+, \lambda^+) = \boldsymbol{x}^{(0)}(k, \lambda|k^+, \lambda^+) + \boldsymbol{K}_{k^+\lambda^+}(k, \lambda|k', \lambda')\boldsymbol{x}(k', \lambda'|k^+, \lambda^+) \tag{5.25}$$

is given as

$$\boldsymbol{x}(k, \lambda|k^+, \lambda^+) = \sum_{n=0}^{\infty}\boldsymbol{K}_{k^+\lambda^+}^n(k, \lambda|k', \lambda')\boldsymbol{x}(k', \lambda'|k^+, \lambda^+). \tag{5.26}$$

We can expand the energy spectrum of the present model with respect to the powers of $1/L$, using the density of roots (5.21)

$$\frac{E}{L} = \frac{1}{L}\sum_{j=1}^{N}(\mu - 2\cos k_j) \tag{5.27}$$

$$= \varepsilon(k^+, \lambda^+) + \frac{1}{L}\varphi(k^+, \lambda^+) - \frac{1}{24L^2}(\epsilon_1(k^+, \lambda^+) + \epsilon_2(k^+, \lambda^+)) + o\left(\frac{1}{L^2}\right) \tag{5.28}$$

where

$$\varepsilon(k^+, \lambda^+) = (\boldsymbol{\varepsilon}_{\rm d}, \boldsymbol{\sigma}^{(0)}) \tag{5.29}$$

$$\varphi(k^+, \lambda^+) = (\boldsymbol{\varepsilon}_{\rm d}, \boldsymbol{\tau}^{(0)}) - \tfrac{1}{2}(\mu - 2) \tag{5.30}$$

and

$$\epsilon_1(k^+, \lambda^+) = \frac{1}{\sigma_L^{\rm c}(k^+|k^+, \lambda^+)}\left(2\sin k^+ - \frac{1}{2}\int_{-k^+}^{k^+} {\rm d}k'\,(\mu - 2\cos k')\rho_1^{\rm c}(k'|k^+, \lambda^+)\right) \tag{5.31}$$

$$\epsilon_2(k^+, \lambda^+) = \frac{1}{\sigma_L^{\rm s}(\lambda^+|k^+, \lambda^+)}\left(-\frac{1}{2}\int_{-k^+}^{k^+} {\rm d}k'\,(\mu - 2\cos k')\rho_2^{\rm c}(k'|k^+, \lambda^+)\right) \tag{5.32}$$

with

$$\boldsymbol{\varepsilon}_0(k, \lambda) = \begin{pmatrix} \mu - 2\cos k \\ 0 \end{pmatrix} \tag{5.33}$$

and

$$\boldsymbol{\varepsilon}_{\rm d}(k, \lambda|k^+, \lambda^+) = \sum_{n=0}^{\infty} \boldsymbol{K}^{{\rm T}\ n}_{k^+,\lambda^+}(k, \lambda|k', \lambda')\boldsymbol{\varepsilon}_0(k', \lambda') \equiv \begin{pmatrix} \varepsilon_{\rm c}(k) \\ \varepsilon_{\rm s}(\lambda) \end{pmatrix}. \tag{5.34}$$

The symbol $\boldsymbol{\varepsilon}_{\rm d}$ denotes the dressed energy of the present model.

If the energy E in the thermodynamic limit is minimized for $k^+ = k^0$ and $\lambda^+ = \lambda^0$, the parameters k^0 and λ^0 are obtained by

$$\frac{\rm d}{{\rm d}k^+}\varepsilon(k^+, \lambda^+) = 0 \qquad \text{and} \qquad \frac{\rm d}{{\rm d}\lambda^+}\varepsilon(k^+, \lambda^+) = 0. \tag{5.35}$$

These relationships are equivalent to

$$\varepsilon_{\rm c}(k^+|k^+, \Lambda^+) = 0 \qquad \text{and} \qquad \varepsilon_{\rm s}(\lambda^+|k^+, \Lambda^+) = 0. \tag{5.36}$$

These equations are the same as the corresponding conditions in the periodic-boundary case. Therefore, we find that $\lambda^0 = \infty$. We remark that the relationships

$$\frac{\rm d}{{\rm d}k^+}\varphi(k^+, \lambda^+) = 0 \qquad \text{and} \qquad \frac{\rm d}{{\rm d}\lambda^+}\varphi(k^+, \lambda^+) = 0. \tag{5.37}$$

also hold for $k^+ = k^0$ and $\lambda^+ = \lambda^0$. Moreover, we find

$$\frac{1}{\sigma_L^{\rm c}(k^0|k^0, \lambda^0)}\frac{{\rm d}^2}{{\rm d}k^{+2}}\varepsilon(k^+, \lambda^+)\bigg|_{\substack{k^+=k^0\\ \lambda^+=\lambda^0}} = \epsilon_1(k^0, \lambda^0)\sigma^{\rm c}(k^0|k^0, \lambda^0) \tag{5.38}$$

and

$$\frac{1}{\sigma_L^{\rm s}(\lambda^0|k^0, \lambda^0)}\frac{{\rm d}^2}{{\rm d}\lambda^{+2}}\varepsilon(k^+, \lambda^+)\bigg|_{\substack{k^+=k^0\\ \lambda^+=\lambda^0}} = \epsilon_2(k^0, \lambda^0)\sigma^{\rm s}(\lambda^0|k^0, \lambda^0). \tag{5.39}$$

Then, we obtain the following form as the expansion of the energy spectrum around the ground state:

$$E = L\varepsilon(\Lambda) + \varphi(\Lambda) + \frac{1}{L}\epsilon_1(k^0,\lambda^0)(\tfrac{1}{2}L^2(k^+ - k^0)^2(\sigma^{\mathrm{c}}(k^0|k^0,\lambda^0))^2 - \tfrac{1}{24}) + \frac{1}{L}\epsilon_2(k^0,\lambda^0)(\tfrac{1}{2}L^2(\lambda^+ - \lambda^0)^2(\sigma^{\mathrm{s}}(\lambda^0|k^0,\lambda^0))^2 - \tfrac{1}{24}) + o\left(\frac{1}{L^2}\right). \tag{5.40}$$

Taking the conditions

$$\int_{-k^+}^{k^+} \sigma_L^{\mathrm{c}}(k)\,\mathrm{d}k = \frac{2N+1}{L} \qquad \text{and} \qquad \int_{-\lambda^+}^{\lambda^+} \sigma_L^{\mathrm{s}}(\lambda)\,\mathrm{d}\lambda = \frac{2M+1}{L} \tag{5.41}$$

into account, we find that the following relationships hold for $k^+ - k^0$ and $\lambda^+ - \lambda^0$ infinitesimal, namely

$$(k^+ - k^0)\sigma^{\mathrm{c}}(k^0|k^0,\lambda^0)L = \frac{1}{\det \boldsymbol{\xi}(k^0,\lambda^0)}((\Delta N - \Theta(p))\xi_{22}(\lambda^0) - (\Delta M - \Theta(p)/2)\xi_{21}(\lambda^0)) \tag{5.42}$$

and

$$(\lambda^+ - \lambda^0)\sigma^{\mathrm{s}}(\lambda^0|k^0,\lambda^0)L = \frac{1}{\det \boldsymbol{\xi}(k^0,\lambda^0)}((\Delta M - \Theta(p)/2)\xi_{11}(k^0) - (\Delta N - \Theta(p))\xi_{12}(k^0)) \tag{5.43}$$

where

$$\Theta(p) \equiv \tfrac{1}{2}\int_{-k^0}^{k^0} \mathrm{d}k\,\theta(k;p) \tag{5.44}$$

with

$$\theta(k;p) = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}k}\theta_0(k;p) + \frac{\cos k}{2\pi}\int_{-k^0}^{k^0} \mathrm{d}k'\,\bar{K}(\sin k - \sin k')\theta(k';p) \tag{5.45}$$

$$\bar{K}(x) = \int_{-\infty}^{+\infty} \mathrm{d}\omega\,\frac{\mathrm{e}^{-u|\omega|}\mathrm{e}^{\mathrm{i}x\omega}}{2\cosh u\omega}. \tag{5.46}$$

Here, the symbols ΔN and ΔM denote the deviations of N and M from their grand-state values, and take integers. The symbols $\{\xi_{ij}\}$ express the dressed charges, which are defined as

$$\boldsymbol{\xi}(k,\lambda) = \sum_{n=0}^{\infty}(\boldsymbol{K}^{\mathrm{T}}_{k^0,\lambda^0})^n \boldsymbol{I} \tag{5.47}$$

where the symbol $\boldsymbol{I}$ denotes the 2×2 identity matrix. Since this definition is the same as that of the corresponding values in the periodic-boundary case, we know that it takes the following form [6]:

$$\begin{pmatrix} \xi_{11}(k^0) & \xi_{12}(k^0) \\ \xi_{21}(\lambda^0) & \xi_{22}(\lambda^0) \end{pmatrix} = \begin{pmatrix} \xi & \xi/2 \\ 0 & 1/\sqrt{2} \end{pmatrix} \qquad \xi \equiv \xi(\sin k^0) \tag{5.48}$$

and

$$\xi(x) = 1 + \frac{1}{2\pi}\int_{-\sin k_0}^{+\sin k_0} \mathrm{d}x'\,\bar{K}(x - x')\xi(x'). \tag{5.49}$$

Here, we evaluate the sound velocities of the present model v_c and v_s, which correspond to the charge sector and the spin sector, respectively. Using the Bethe ansatz equations (3.21) and (3.22), we obtain the following relationship:

$$\sum_{j=-N}^{N} k_j = \pi \sum_{j=-N}^{N} \frac{I_j}{L} + \pi \sum_{\beta=-M}^{M} \frac{J_\beta}{L}. \tag{5.50}$$

From this equation, we can recognize the dressed momenta $p_c(k_j)$ as $\pi I_j/L$ and $p_s(\lambda_\beta)$ as $\pi J_\beta/L$. Therefore, we can evaluate the sound velocities as

$$v_c = \left.\frac{d\varepsilon_c(k)}{dp_c(k)}\right|_{k=k^0} = \frac{\epsilon_1(k^0, \lambda^0)}{\pi} \tag{5.51}$$

$$v_s = \left.\frac{d\varepsilon_s(\lambda)}{dp_s(\lambda)}\right|_{\lambda=\lambda^0} = \frac{\epsilon_2(k^0, \lambda^0)}{\pi}. \tag{5.52}$$

These velocities equal those of the system with the periodic boundary condition [6].

Summing up the above discussions, we express the energy spectrum around the ground state as

$$E(\Delta N, \Delta\tilde{M}) = Le_\infty + f_\infty + \frac{\pi v_c}{L}\left\{\frac{1}{2}\frac{(\Delta N - \Theta(p))^2}{\xi^2} - \frac{1}{24}\right\} + \frac{\pi v_s}{L}\left\{\frac{1}{2}\frac{(\Delta\tilde{M})^2}{(1/\sqrt{2})^2} - \frac{1}{24}\right\} + o\left(\frac{1}{L}\right) \tag{5.53}$$

where

$$e_\infty = \varepsilon(k^0, \lambda^0) \qquad \text{and} \qquad f_\infty = \varphi(k^0, \lambda^0) \tag{5.54}$$

and

$$\Delta\tilde{M} = \Delta M - \tfrac{1}{2}\Delta N. \tag{5.55}$$

In order to obtain the complete form of the low-lying spectrum, we consider a particle–hole excitation in the vicinity of the Fermi surface. In each sector, we describe each particle–hole pair as

$$z_L^c(k_p) = \frac{I_p}{L} \qquad \text{and} \qquad z_L^c(k_h) = \frac{I_h}{L} \tag{5.56}$$

$$z_L^s(\lambda_p) = \frac{J_p}{L} \qquad \text{and} \qquad z_L^s(\lambda_h) = \frac{J_h}{L}. \tag{5.57}$$

By introducing the following half-odd numbers n_p^c and n_h^c, n_p^s and n_h^s,

$$I_p = I^+ + \tfrac{1}{2} + n_p^c \qquad \text{and} \qquad I_h = I^+ + \tfrac{1}{2} - n_h^c \tag{5.58}$$

$$J_p = J^+ + \tfrac{1}{2} + n_p^s \qquad \text{and} \qquad J_h = J^+ + \tfrac{1}{2} - n_h^s \tag{5.59}$$

we characterize each particle–hole excitation by the positive integers

$$n_{ph}^c \equiv n_p^c + n_h^c \qquad \text{and} \qquad n_{ph}^s \equiv n_p^s + n_h^s. \tag{5.60}$$

Since the presence of these particle–hole pairs modifies $\boldsymbol{\sigma}_L$ by

$$-\frac{k_p - k_h}{L}\boldsymbol{\rho}_1(k, \lambda | k^+, \lambda^+) - \frac{\lambda_p - \lambda_h}{L}\boldsymbol{\rho}_2(k, \lambda | k^+, \lambda^+) \tag{5.61}$$

this excitation changes the energy by

$$\frac{n_{ph}^c}{L}\epsilon_1(k^+, \lambda^+) + \frac{n_{ph}^s}{L}\epsilon_2(k^+, \lambda^+). \tag{5.62}$$

If several particle–hole pairs exist, we have to replace $n^{\rm c}_{\rm ph}$ and $n^{\rm s}_{\rm ph}$ by the non-negative integers $N^{\rm c}_+$ and $N^{\rm s}_+$ defined as

$$N^{\rm c}_+ = \sum_{\text{all pairs}} n^{\rm c}_{\rm ph} \qquad \text{and} \qquad N^{\rm s}_+ = \sum_{\text{all pairs}} n^{\rm s}_{\rm ph}. \tag{5.63}$$

Finally, we obtain the energy spectrum around the ground state as

$$E(\Delta N, \Delta\tilde{M}, N^{\rm c}_+, N^{\rm s}_+) = Le_\infty + f_\infty + \frac{\pi v_{\rm c}}{L}\left\{\frac{1}{2}\frac{(\Delta N - \Theta(p))^2}{\xi^2} - \frac{1}{24} + N^{\rm c}_+\right\} + \frac{\pi v_{\rm s}}{L}\left\{\frac{1}{2}\frac{(\Delta\tilde{M})^2}{(1/\sqrt{2})^2} - \frac{1}{24} + N^{\rm s}_+\right\} + o\left(\frac{1}{L}\right). \tag{5.64}$$

Here, ΔN and $\Delta\tilde{M}$ take integers and $N^{\rm c}_+$ and $N^{\rm s}_+$ take non-negative integers. For a given $N^{\rm c}_+$ ($N^{\rm s}_+$), the degeneracy is given by Euler's partition number $P(N^{\rm c}_+)$ ($P(N^{\rm s}_+)$).

6. Partition functions

In the present section, we evaluate the following partition function for each model in the scaling limit

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\hat{H}/T} \tag{6.1}$$

where $\hat{H}$ is defined as

$$\hat{H} \equiv \mathcal{H} - e_\infty L - f_\infty. \tag{6.2}$$

First, we discuss the XXZ model with a boundary field. By using equation (4.53), we obtain the partition function in the scaling limit $q \equiv \exp(-\pi v_{\rm s}/TL) \sim 0$ as follows,

$$Z_{XXZ} = q^{-1/24} \sum_{\Delta M \in \mathbb{Z}} q^{(\Delta M - \Theta)^2/2\xi^2} \sum_{N_+=0}^{\infty} P(N_+) q^{N_+}. \tag{6.3}$$

Here, the degeneracy for a given N_+ is described by Euler's partition number $P(N_+)$. Therefore, we can rewrite the partition function in the following form:

$$Z_{XXZ} = \frac{1}{\eta(q)} \sum_{\Delta M \in \mathbb{Z}} q^{(\Delta M - \Theta)^2/2\xi^2} \tag{6.4}$$

where

$$\eta(q) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n) \tag{6.5}$$

which is Dedekind's η-function.

In the same way, by using equation (5.64), we obtain the partition function of each sector in the Hubbard model in the scaling limit $q_{\rm c} \equiv \exp(-\pi v_{\rm c}/TL) \sim 0$ and $q_{\rm s} \equiv \exp(-\pi v_{\rm s}/TL) \sim 0$ as follows:

$$Z_{\rm c} = \frac{1}{\eta(q_{\rm c})} \sum_{\Delta N \in \mathbb{Z}} q_{\rm c}^{(\Delta N - \Theta)^2/2\xi^2} \tag{6.6}$$

$$Z_{\rm s} = \frac{1}{\eta(q_{\rm s})} \sum_{\Delta\tilde{M} \in \mathbb{Z}} q_{\rm s}^{(\Delta\tilde{M})^2/2(1/\sqrt{2})^2}. \tag{6.7}$$

When $\gamma \to \pi/2$ in equation (2.2), the XXZ model approaches the XX model. The XX model with a boundary field can be solved by using the Jordan–Wigner transformation instead of the Bethe ansatz, so that its partition function is evaluated [14]. We can confirm that the partition function of the XXZ model becomes that of the XX model, namely

$$Z_{XXZ}(p; \gamma = \pi/2) = Z_{XX}(p). \tag{6.8}$$

(We note that in the present paper the definitions of the boundary field and the function Θ are different from those in our previous work [14].) On the other hand, when $\gamma \to 0$ in equation (2.2), the XXZ model approaches the antiferromagnetic XXX model. Then, we find

$$Z_{XXZ}(p = 0; \gamma = 0) = Z_{\mathrm{s}}. \tag{6.9}$$

This relationship is plausible, since the spin sector of the Hubbard model has the $SU(2)$ invariance even if U is not infinite or the filling is not half.

7. Conformal weights and surface exponents

In the present section, we discuss operator contents in the present models. We also evaluate the surface critical exponents of the corresponding classical systems.

At first, we remark that each sector of these models gives a representation of the shifted $U(1)$ Kac–Moody algebra [15] with $c = 1$. As was discussed in our previous work [14], we can construct a representation of the algebra by using the chiral Gaussian field so that we can calculate the partition function as

$$Z_{\mathrm{G}}(R; \theta) = \sum_{M \in \mathbb{Z}} \chi_{M/R}(\theta) \qquad \chi_\phi \equiv \frac{1}{\eta(q)} q^{(\phi+\theta)^2/2} \tag{7.1}$$

where R denotes a quantization radius of the field and takes a positive number. For the detailed derivation, see [14]. We describe the character of the irreducible representation in the algebra by $\chi_\phi(\theta)$, which corresponds to the primary field with the conformal weight [15]

$$\Delta(\phi, \theta) = \tfrac{1}{2}(\phi + \theta)^2. \tag{7.2}$$

Therefore, we obtain the conformal dimensionality of each primary field in the present Gaussian field as follows [14]:

$$\Delta^{\mathrm{G}}_M(R; \theta) = \frac{1}{2}\left(\frac{M}{R} + \theta\right)^2 \qquad M \in \mathbb{Z}. \tag{7.3}$$

We compare Z_{G} with the partition functions obtained in the preceding sections to obtain

$$Z_{XXZ} = Z_{\mathrm{G}}(R = \xi; \theta = \Theta/\xi) \tag{7.4}$$

$$Z_{\mathrm{c}} = Z_{\mathrm{G}}(R = \xi; \theta = \Theta/\xi) \tag{7.5}$$

$$Z_{\mathrm{s}} = Z_{\mathrm{G}}(R = 1/\sqrt{2}; \theta = 0). \tag{7.6}$$

Note the definitions of the ξ's and Θ's, which are different from each other. These relationships mean that each sector of these models gives a representation of the (shifted) $U(1)$ Kac–Moody algebra with $c = 1$. The conformal weight of each primary field contained in these sectors is given by

$$\Delta_{XXZ}(n) = \Delta^{\mathrm{G}}_n(R = \xi; \theta = \Theta/\xi) = \frac{1}{2}\frac{(n+\Theta)^2}{\xi^2} \tag{7.7}$$

$$\Delta_{\mathrm{c}}(n) = \Delta^{\mathrm{G}}_n(R = \xi; \theta = \Theta/\xi) = \frac{1}{2}\frac{(n+\Theta)^2}{\xi^2} \tag{7.8}$$

$$\Delta_{\mathrm{s}}(n) = \Delta^{\mathrm{G}}_n(R = 1/\sqrt{2}; \theta = 0) = n^2 \tag{7.9}$$

where n takes integers. We find that the conformal weights in the present XXZ model and the charge sector of the Hubbard model vary depending on the boundary fields.

According to Cardy's argument [13], we can evaluate the surface critical exponent x_{s} in the corresponding classical system by the following relationship:

$$E_1 - E_0 = \frac{\pi v}{L} x_{\mathrm{s}} \tag{7.10}$$

where the symbols E_0 and E_1 denote the ground-state energy and the first excited energy, respectively, and v denotes the Fermi velocity in each sector. Taking equations (4.53) and (5.64) into account, we evaluate the energies of each sector of the present models to obtain the following common form:

$$E_1 - E_0 = \frac{\pi v}{L} \left\{ \frac{1}{2} \left(\frac{1}{R} - |\theta| \right)^2 - \frac{1}{2} \theta^2 \right\} \tag{7.11}$$

apart from the higher order corrections. Thus, we obtain

$$x_{\mathrm{s}} = \frac{1}{2} \left(\frac{1}{R^2} - \frac{2|\theta|}{R} \right). \tag{7.12}$$

When the parameter θ changes, depending on the boundary field, the exponent varies as a function of the field.

8. Summary

We have found that each of the following sectors gives a representation of the shifted $U(1)$ Kac–Moody algebra with $c = 1$:

- the XXZ model with the boundary field;
- the charge sector of the Hubbard model with the boundary field;
- the spin sector of the Hubbard model with the boundary field.

In each case, the parameter θ of the algebra is given as a function of the boundary field. When the field vanishes, θ becomes zero. On the other hand, the parameter θ in the spin sector of the present Hubbard model equals zero even if the boundary field is finite. This is a plausible result, because the boundary field of the Hubbard model does not depend on the spin of a particle. The conformal dimensions of the primary fields of the XXZ model and the charge sector in the Hubbard model change as functions of the boundary fields. The surface critical exponents also depend on the boundary field through the parameter θ.

We have also discussed the operator contents of the supersymmetric t–J model with a boundary field. The results will be given elsewhere [20].

Appendix

In the present section, we explain how to derive equation (3.16) by giving examples using a few particles. These examples allow us confirm the validity of the Bethe ansatz wavefunction (3.2).

We describe a base which spans the Hilbert space of the model (3.1) with N particles as

$$|x_1\sigma_1, x_2\sigma_2, \ldots, x_N\sigma_N\rangle \equiv c^{\dagger}_{x_1\sigma_1} c^{\dagger}_{x_2\sigma_2} \ldots c^{\dagger}_{x_N\sigma_N} |0\rangle \tag{A.1}$$

where the symbol $|0\rangle$ denotes the vacuum. We can express the wavefunction (eigenfunction) $\psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N)$ corresponding to the state vector (eigenvector) $|\psi\rangle$ with N particles, in the following way:

$$\psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N) = \langle x_1\sigma_1,\ldots,x_N\sigma_N|\psi\rangle \tag{A.2}$$

namely

$$|\psi\rangle = \sum_{\{(x_j,\sigma_j)\}} \psi_{\sigma_1,\ldots,\sigma_N}(x_1,\ldots,x_N)|x_1\sigma_1,\ldots,x_N\sigma_N\rangle. \tag{A.3}$$

Then, the following eigenvalue equation holds:

$$\mathcal{H}|\psi\rangle = E|\psi\rangle \tag{A.4}$$

where the Hamiltonian $\mathcal{H}$ is defined in (3.1) and E denotes the energy eigenvalue of the present model. In the present section, we omit the chemical potential μ from the Hamiltonian (3.1) for simplicity. Since the numbers of up-spin particles and down-spin particles are conserved quantities in the present model, we can add the contributions from not only the chemical potential $\mu\sum_{j=1}^{L}(n_{j+}+n_{j-})$ but also the magnetic field $h\sum_{j=1}^{L}(n_{j+}-n_{j-})$ to the energy eigenvalue after solving the present model.

First, we discuss the case with $N=1$. The eigenvalue equation (A.4) yields the following three equations:

$$E\psi_\sigma(x) = -\psi_\sigma(x+1) - \psi_\sigma(x-1) \qquad \text{for } x = 2,\ldots,L-1 \tag{A.5}$$

$$E\psi_\sigma(1) = -p_\sigma\psi_\sigma(1) - \psi_\sigma(2) \tag{A.6}$$

$$E\psi_\sigma(L) = -p_\sigma\psi_\sigma(L) - \psi_\sigma(L-1). \tag{A.7}$$

We assume the form of the eigenfunction as

$$\psi_\sigma(x) = A_\sigma(k)\mathrm{e}^{\mathrm{i}kx} - A_\sigma(k)\mathrm{e}^{-\mathrm{i}kx} \tag{A.8}$$

which corresponds to the wavefunction (3.2) with $N=1$. From equation (A.5) we obtain

$$E = -2\cos k. \tag{A.9}$$

Substituting this value of E into equations (A.6) and (A.7), we can derive the following relationships:

$$A_\sigma(k)(1-p_\sigma\mathrm{e}^{\mathrm{i}k}) - A_\sigma(-k)(1-p_\sigma\mathrm{e}^{-\mathrm{i}k}) = 0 \tag{A.10}$$

$$A_\sigma(k)(1-p_\sigma\mathrm{e}^{-\mathrm{i}k})\mathrm{e}^{\mathrm{i}k(L+1)} - A_\sigma(-k)(1-p_\sigma\mathrm{e}^{\mathrm{i}k})\mathrm{e}^{-\mathrm{i}k(L+1))} = 0 \tag{A.11}$$

respectively. We can rewrite these equations as follows:

$$A_\sigma(-k) = s^{\mathrm{L}}(k;p_\sigma)A_\sigma(k) \tag{A.12}$$

and

$$A_\sigma(-k) = s^{\mathrm{R}}(k;p_\sigma)A_\sigma(k) \tag{A.13}$$

respectively, where the symbols s^{L} and s^{R} are defined in equation (3.8). The equations (A.12) and (A.13) correspond to the relationships (3.5) and (3.6) with $N=1$. Then compatibility between (A.12) and (A.13) yields

$$s^{\mathrm{L}}(k;p_\sigma) = s^{\mathrm{R}}(k;p_\sigma) \tag{A.14}$$

or, using (3.8) and (3.9),

$$s^2(k;p_\sigma)\mathrm{e}^{\mathrm{i}k2(L+1)} = 1. \tag{A.15}$$

This relationship is nothing but equation (3.16) with $N=1$.

Next, we discuss the case with $N = 2$. We consider the following wavefunction with $N = 2$:

$$\psi_{\sigma_1,\sigma_2}(x_1, x_2) = \sum_P \varepsilon_P A_{\sigma_{Q1},\sigma_{Q2}}(k_{PQ1}, k_{PQ2}) \mathrm{e}^{\mathrm{i}k_{P1}x_1 + \mathrm{i}k_{P2}x_2} \tag{A.16}$$

where

$$1 \leqslant x_{Q1} \leqslant x_{Q2} \leqslant L. \tag{A.17}$$

The sum extends over the permutations and the negations of k_1 and k_2, and ε_P denotes a sign factor (± 1) that changes its sign at each such 'mutation'. For $N = 2$, we consider two sectors $x_1 \leqslant x_2$ and $x_2 \leqslant x_1$. Corresponding to these sectors, we take I (identity) and X (exchange) as the permutation Q in the wavefunction (A.16). As an example, we explicitly write the wavefunction with $Q = I$:

$$\begin{aligned}\psi^I_{\sigma_1,\sigma_2}(x_1, x_2) = {} & A_{\sigma_1,\sigma_2}(k_1, k_2)\mathrm{e}^{\mathrm{i}k_1x_1+\mathrm{i}k_2x_2} - A_{\sigma_1,\sigma_2}(k_1, -k_2)\mathrm{e}^{\mathrm{i}k_1x_1-\mathrm{i}k_2x_2} \\ & -A_{\sigma_1,\sigma_2}(-k_1, k_2)\mathrm{e}^{-\mathrm{i}k_1x_1+\mathrm{i}k_2x_2} + A_{\sigma_1,\sigma_2}(-k_1, -k_2)\mathrm{e}^{-\mathrm{i}k_1x_1-\mathrm{i}k_2x_2} \\ & -A_{\sigma_1,\sigma_2}(k_2, k_1)\mathrm{e}^{\mathrm{i}k_2x_1+\mathrm{i}k_1x_2} + A_{\sigma_1,\sigma_2}(k_2, -k_1)\mathrm{e}^{\mathrm{i}k_2x_1-\mathrm{i}k_1x_2} \\ & +A_{\sigma_1,\sigma_2}(-k_2, k_1)\mathrm{e}^{-\mathrm{i}k_2x_1+\mathrm{i}k_1x_2} - A_{\sigma_1,\sigma_2}(-k_2, -k_1)\mathrm{e}^{-\mathrm{i}k_2x_1-\mathrm{i}k_1x_2}.\end{aligned} \tag{A.18}$$

Similarly, the wavefunction with $Q = X$ can also be described as a summation of eight 'mutant replicas', according to the definition. Then, the relationship

$$\psi^I_{\sigma_1,\sigma_2}(x, x) = \psi^X_{\sigma_1,\sigma_2}(x, x) \tag{A.19}$$

must be satisfied. For this purpose, we assume that the condition

$$A_{\sigma_1,\sigma_2}(k_1, k_2) - A_{\sigma_1,\sigma_2}(k_2, k_1) = A_{\sigma_2,\sigma_1}(k_2, k_1) - A_{\sigma_2,\sigma_1}(k_1, k_2) \tag{A.20}$$

together with its 'mutant' conditions hold, which are obtained by replacing k_1 with $-k_1$ or k_2 with $-k_2$.

The eigenvalue equation (A.4) yields some kind of equations, namely

$$\begin{aligned}E\psi_{\sigma_1,\sigma_2}(x_1, x_2) = {} & -\psi_{\sigma_1,\sigma_2}(x_1 - 1, x_2) - \psi_{\sigma_1,\sigma_2}(x_1 + 1, x_2) - \psi_{\sigma_1,\sigma_2}(x_1, x_2 - 1) \\ & -\psi_{\sigma_1,\sigma_2}(x_1, x_2 + 1) \qquad \text{for } x_1 \neq x_2,\ 2 \leqslant x_1 \leqslant L - 1 \text{ and } 2 \leqslant x_2 \leqslant L - 1\end{aligned} \tag{A.21}$$

$$\begin{aligned}E\psi_{\sigma_1,\sigma_2}(x, x) = {} & -\psi_{\sigma_1,\sigma_2}(x - 1, x) - \psi_{\sigma_1,\sigma_2}(x + 1, x) - \psi_{\sigma_1,\sigma_2}(x, x - 1) \\ & -\psi_{\sigma_1,\sigma_2}(x, x + 1) + U\psi_{\sigma_1,\sigma_2}(x, x) \qquad \text{for } 2 \leqslant x \leqslant L - 1\end{aligned} \tag{A.22}$$

$$\begin{aligned}E\psi_{\sigma_1,\sigma_2}(1, x) = {} & -\psi_{\sigma_1,\sigma_2}(2, x) - \psi_{\sigma_1,\sigma_2}(1, x - 1) - \psi_{\sigma_1,\sigma_2}(1, x + 1) - p_{\sigma_1}\psi_{\sigma_1,\sigma_2}(1, x) \\ & \text{for } 2 \leqslant x \leqslant L - 1\end{aligned} \tag{A.23}$$

$$\begin{aligned}E\psi_{\sigma_1,\sigma_2}(x, L) = {} & -\psi_{\sigma_1,\sigma_2}(x - 1, L) - \psi_{\sigma_1,\sigma_2}(x + 1, L) - \psi_{\sigma_1,\sigma_2}(x, L - 1) \\ & -p_{\sigma_2}\psi_{\sigma_1,\sigma_2}(x, L) \qquad \text{for } 2 \leqslant x \leqslant L - 1\end{aligned} \tag{A.24}$$

and other equations which correspond to equation (A.4) with $2 \leqslant x_1 \leqslant L - 1$ and $x_2 = 1$, $x_1 = L$ and $2 \leqslant x_2 \leqslant L - 1$, $x_1 = 1$ and $x_2 = L$, $x_1 = L$ and $x_2 = 1$, $x_1 = x_2 = 1$, and $x_1 = x_2 = L$. Substituting the wavefunction (A.16) into equation (A.21), we obtain

$$E = -2 \sum_{j=1,2} \cos k_j. \tag{A.25}$$

The eigenvalue equations (A.22)–(A.24) with the eigenvalue E (A.25) hold, when the following conditions are satisfied:

$$A_{\sigma_2,\sigma_1}(k_2,k_1) = \frac{\sin k_1 - \sin k_2}{\sin k_1 - \sin k_2 + \mathrm{i}U/2} A_{\sigma_1,\sigma_2}(k_1,k_2) + \frac{\mathrm{i}U/2}{\sin k_1 - \sin k_2 + \mathrm{i}U/2} A_{\sigma_2,\sigma_1}(k_1,k_2) \tag{A.26}$$

$$A_{\sigma_i,\sigma_j}(k_1,k_2)(1 - p_{\sigma_i}\mathrm{e}^{\mathrm{i}k_1}) = A_{\sigma_i,\sigma_j}(-k_1,k_2)(1 - p_{\sigma_i}\mathrm{e}^{-\mathrm{i}k_1}) \tag{A.27}$$

$$A_{\sigma_i,\sigma_j}(k_1,k_2)(1 - p_{\sigma_j}\mathrm{e}^{-\mathrm{i}k_2})\mathrm{e}^{\mathrm{i}k_2(L+1)} = A_{\sigma_i,\sigma_j}(k_1,-k_2)(1 - p_{\sigma_j}\mathrm{e}^{\mathrm{i}k_2})\mathrm{e}^{-\mathrm{i}k_2(L+1)}$$
$$\text{for } i = 1,2, \quad j = 1,2 \text{ and } i \neq j \tag{A.28}$$

together with their 'mutant' conditions which can be obtained from (A.26) by negations of $\{k_1, k_2\}$ and from (A.27) and (A.28) by permutations or negations of $\{k_1, k_2\}$. Here, we have used the condition (A.20) for these derivations. We can confirm that the other equations written below equation (A.24) also hold when these conditions are satisfied. We can rewrite the relationships (A.26)–(A.28) as follows:

$$A_{\sigma_2,\sigma_1}(k_2,k_1) = S_{12}(k_1,k_2)A_{\sigma_1,\sigma_2}(k_1,k_2) \tag{A.29}$$

$$A_{\sigma_i,\sigma_j}(-k_1,k_2) = s^{\mathrm{L}}(k_1; p_{\sigma_i})A_{\sigma_i,\sigma_j}(k_1,k_2) \tag{A.30}$$

and

$$A_{\sigma_i,\sigma_j}(k_1,-k_2) = s^{\mathrm{R}}(k_2; p_{\sigma_j})A_{\sigma_i,\sigma_j}(k_1,k_2) \tag{A.31}$$

where the definitions of S_{12}, s^{L} and s^{R} are given by equations (3.7)–(3.9). Using these relationships successively, we can derive the following equation:

$$A_{\sigma_1,\sigma_2}(k_1,k_2) = s^{\mathrm{L}}(-k_1; p_{\sigma_1})A_{\sigma_1}(-k_1,k_2) = s^{\mathrm{L}}(-k_1; p_{\sigma_1})S_{21}(k_2,-k_1)A_{\sigma_1}(k_2,-k_1) = \cdots$$
$$\cdots = s^{\mathrm{L}}(-k_1; p_{\sigma_1})S_{21}(k_2,-k_1)s^{\mathrm{R}}(k_1; p_{\sigma_1})S_{12}(k_1,k_2)A_{\sigma_1,\sigma_2}(k_1,k_2) \tag{A.32}$$

namely,

$$A_{\sigma_1,\sigma_2}(k_1,k_2) = T_1 A_{\sigma_1,\sigma_2}(k_1,k_2) \tag{A.33}$$

where T_1 is defined in equation (3.11). In the same way, we can derive the equation

$$A_{\sigma_1,\sigma_2}(k_1,k_2) = T_2 A_{\sigma_1,\sigma_2}(k_1,k_2). \tag{A.34}$$

Then, we obtain the eigenvalue equations to solve as follows

$$T_j \boldsymbol{t} = 1 \times \boldsymbol{t} \qquad j = 1,2 \tag{A.35}$$

where the symbol $\boldsymbol{t}$ denotes an eigenvector on the space of the spin variables. This set of equations is just the same as equation (3.16) with $N = 2$.

Finally, we discuss the case with general N. The eigenvalue equation (A.4) yields

$$E\langle x_1\sigma_1, \ldots, x_N\sigma_N|\psi\rangle = \langle x_1\sigma_1, \ldots, x_N\sigma_N|\mathcal{H}|\psi\rangle. \tag{A.36}$$

For $\{x_j\}$ not taking 1 or L, we can confirm that the wavefunction (3.2) satisfies equation (A.36) with the eigenvalue

$$E = -2\sum_{j=1}^{N} \cos k_j \tag{A.37}$$

using the relationship (3.4) together with its 'mutant' relationships, similar to the periodic-boundary case. When x_j takes 1 or L for $^{\exists}j$, some terms coupling the boundary field, namely

$$-p_{\sigma_j}\psi_{\sigma_1,\ldots,\sigma_N}(\ldots, x_j = 1, \ldots) \qquad \text{or} \qquad -p_{\sigma_j}\psi_{\sigma_1,\ldots,\sigma_N}(\ldots, x_j = L, \ldots) \tag{A.38}$$

emerge on the right-hand side of equation (A.36), as shown in (A.23) or (A.24) for example. If the relationships (3.5) and (3.6) together with their 'mutant' relationships are satisfied, the following relationships hold:

$$p_{\sigma_j}\psi_{\sigma_1,\ldots,\sigma_N}(\ldots,x_j=1,\ldots)=\psi_{\sigma_1,\ldots,\sigma_N}(\ldots,x_j=0,\ldots) \tag{A.39}$$

and

$$p_{\sigma_j}\psi_{\sigma_1,\ldots,\sigma_N}(\ldots,x_j=L,\ldots)=\psi_{\sigma_1,\ldots,\sigma_N}(\ldots,x_j=L+1,\ldots) \tag{A.40}$$

where $\psi_{\sigma_1,\ldots,\sigma_N}(\ldots,x_j = 0,\ldots)$ and $\psi_{\sigma_1,\ldots,\sigma_N}(\ldots,x_j = L+1,\ldots)$ are defined by equation (3.2) with $x_j = 0$ and $x_j = L+1$, respectively. Then, we can recognize the present system with boundary fields as a system with two virtual sites '0' and '$L+1$' without boundary fields. We note that each of the virtual sites is not doubly occupied. This kind of trick has been used by Alcaraz *et al* [16] in solving the XXZ model with boundary fields. After this interpretation, we can check that the wavefunction (3.2) satisfies equation (A.36) under the condition (3.4), similar to the periodic-boundary case. In this way, we can derive the eigenvalue equation (3.16) for any N.

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