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ScienceDirect
Nuclear Physics B 879 [FS] (2014) 98–109
NUCLEAR PHYSICS B
www.elsevier.com/locate/nuclphysb

Exact solution of the one-dimensional Hubbard model with arbitrary boundary magnetic fields

Yuan-Yuan Li [a], Junpeng Cao [a], Wen-Li Yang [b,c], Kangjie Shi [b], Yupeng Wang [a,*]

[a] *Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[b] *Institute of Modern Physics, Northwest University, Xian 710069, China*

[c] *Beijing Center for Mathematics and Information Interdisciplinary Sciences, Beijing, 100048, China*

Received 10 November 2013; accepted 5 December 2013

Available online 11 December 2013

Abstract

The one-dimensional Hubbard model with arbitrary boundary magnetic fields is solved exactly via the Bethe ansatz methods. With the coordinate Bethe ansatz in the charge sector, the second eigenvalue problem associated with the spin sector is constructed. It is shown that the second eigenvalue problem can be transformed into that of the inhomogeneous XXX spin chain with arbitrary boundary fields which can be solved via the off-diagonal Bethe ansatz method.

Keywords: Hubbard model; Bethe ansatz; T–Q relation

1. Introduction

The Hubbard model is one of the essential models in condensed matter physics. An interesting issue is that the model is exactly solvable in one dimension [1], which provides an important benchmark for understanding the Mott insulators. After Lieb and Wu's pioneering work, a lot of attentions have been paid to the integrability, symmetry [2–5] and physical properties of this

* Corresponding author.
E-mail address: yupeng@iphy.ac.cn (Y. Wang).

http://dx.doi.org/10.1016/j.nuclphysb.2013.12.004

model. A remarkable result was obtained by Shastry [6] and by Olmedilla et al. [7,8] who constructed the corresponding R-matrix of the one-dimensional Hubbard model and therefore demonstrated its complete integrability in the framework of Yang–Baxter equation [9,10]. Subsequently, the model was resolved [11] via the algebraic Bethe ansatz method based on the result of Shastry. Another interesting issue about this model is the open-boundary problem, which is tightly related to the impurity problem in a Luttinger liquid [12]. The exact solution of the open Hubbard chain was firstly obtained by Shulz [13]. Subsequently, the exact solution of the model with boundary potentials was obtained [14,15]. The integrability of the one-dimensional Hubbard model with diagonal open boundary was demonstrated in [16] by constructing the Lax representation and solved by algebraic Bethe ansatz method [17]. The generic integrable boundary conditions were obtained in [18] by solving the reflection equation [19–21]. It was found [18] that in the spin sector magnetic fields applied on the two end sites do not break the integrability of this model. Although the integrability has been known for long time, the exact solutions (or diagonalization of the Hamiltonian) of the model with arbitrary boundary magnetic fields are still lacking.

In this paper, we study the open Hubbard chain with arbitrary boundary magnetic fields. The Hamiltonian of the model is

$$H = -t \sum_{\alpha, j=1}^{N-1} \left[c_{j,\alpha}^{\dagger} c_{j+1,\alpha} + c_{j+1,\alpha}^{\dagger} c_{j,\alpha}\right] + U \sum_{j=1}^{N} n_{j,\uparrow} n_{j,\downarrow} + h_1^- c_{1,\uparrow}^{\dagger} c_{1,\downarrow} + h_1^+ c_{1,\downarrow}^{\dagger} c_{1,\uparrow} + h_1^z (n_{1,\uparrow} - n_{1,\downarrow}) + h_N^- c_{N,\uparrow}^{\dagger} c_{N,\downarrow} + h_N^+ c_{N,\downarrow}^{\dagger} c_{N,\uparrow} + h_N^z (n_{N,\uparrow} - n_{N,\downarrow}), \tag{1.1}$$

where $c_{j,\alpha}^{\dagger}$ and $c_{j,\alpha}$ are the creation and annihilation operators of electrons on site j with spin component $\alpha = \uparrow, \downarrow$; t and U are the hopping constant and the on-site repulsion constant as usual; $n_{j,\alpha}$ are particle number operators, respectively; $\vec{h}_1 = (h_1^x, h_1^y, h_1^z)$ and $\vec{h}_N = (h_N^x, h_N^y, h_N^z)$ indicate the boundary fields and $h_j^{\pm} = h_j^x \pm i h_j^y$ for $j = 1, N$. We shall show in the following that the model can be exactly solved by combining the coordinate Bethe ansatz and the off-diagonal Bethe ansatz proposed recently in [22–24] for arbitrary $\vec{h}_1$ and $\vec{h}_N$. We remark that the unparallel boundary fields break the $U(1)$ symmetry in spin sector and make the total spin no longer a conserved charge.

The paper is organized as follows. In Section 2, we use the coordinate Bethe ansatz method to derive the eigenvalue equation in the spin sector as that in the periodic case [9]. In Section 3, we transform this eigenvalue problem into that of the inhomogeneous XXX spin chain with boundary fields, which allows us to apply the recently proposed off-diagonal Bethe ansatz method [22–24] to solve it. The exact spectrum of the Hamiltonian and the Bethe ansatz equations are thus obtained. Section 4 is attributed to the reduction to the parallel or anti-parallel boundary case. Concluding remarks are given in Section 5.

2. Coordinate Bethe ansatz

Though the $U(1)$ symmetry in the spin sector is broken by the unparallel boundary fields, the $U(1)$ symmetry in the charge sector is still reserved. The conserved charge corresponding to this reserved symmetry is the total number operator of electrons, namely,

$$\hat{N} = \sum_{j=1}^{N} \{n_{j,\uparrow} + n_{j,\downarrow}\}, \quad [H, \hat{N}] = 0. \tag{2.1}$$

The symmetry allows us to construct the eigenstate of the Hamiltonian (1.1) with a fixed number of electrons as follows:

$$|\Psi\rangle = \sum_{j=1}^{M} \sum_{\alpha_j=\uparrow,\downarrow} \sum_{x_j=1}^{N} \Psi^{\{\alpha\}}(x_1,\ldots,x_M) c^{\dagger}_{x_1,\alpha_1}\cdots c^{\dagger}_{x_M,\alpha_M}|0\rangle, \tag{2.2}$$

where M is the number of electrons and $\{\alpha\} = (\alpha_1,\ldots,\alpha_M)$. The eigenvalue equation of the Hamiltonian then reads

$$\begin{aligned}
&-t\sum_{j=1}^{M}\big[(1-\delta_{x_j,N})\Psi^{\{\alpha\}}(\ldots,x_j+1,\ldots)+(1-\delta_{x_j,1})\Psi^{\{\alpha\}}(\ldots,x_j-1,\ldots)\big]\\
&\quad + U\sum_{i<j}^{M}\delta_{x_i,x_j}\delta_{\alpha_i,-\alpha_j}\Psi^{\{\alpha\}}(x_1,\ldots,x_M)\\
&\quad + \sum_{j=1}^{M}\delta_{x_j,1}\big[h_1^-\delta_{\alpha_j,\downarrow}\Psi^{(\ldots,-\alpha_j,\ldots)}(x_1,\ldots,x_M)+h_1^+\delta_{\alpha_j,\uparrow}\Psi^{(\ldots,-\alpha_j,\ldots)}(x_1,\ldots,x_M)\\
&\quad + h_1^z(\delta_{\alpha_j,\uparrow}-\delta_{\alpha_j,\downarrow})\Psi^{\{\alpha\}}(x_1,\ldots,x_M)\big]\\
&\quad + \sum_{j=1}^{M}\delta_{x_j,N}\big[h_N^-\delta_{\alpha_j,\downarrow}\Psi^{(\ldots,-\alpha_j,\ldots)}(x_1,\ldots,x_M)+h_N^+\delta_{\alpha_j,\uparrow}\Psi^{(\ldots,-\alpha_j,\ldots)}(x_1,\ldots,x_M)\\
&\quad + h_N^z(\delta_{\alpha_j,\uparrow}-\delta_{\alpha_j,\downarrow})\Psi^{\{\alpha\}}(x_1,\ldots,x_M)\big]\\
&= E\,\Psi^{\{\alpha\}}(x_1,\ldots,x_M).
\end{aligned} \tag{2.3}$$

This eigenvalue equation can be rewritten as

$$\begin{aligned}
&-t\sum_{j=1}^{M}\big[(1-\delta_{x_j,N})\Psi^{\{\alpha\}}(\ldots,x_j+1,\ldots)+(1-\delta_{x_j,1})\Psi^{\{\alpha\}}(\ldots,x_j-1,\ldots)\big]\\
&\quad + U\sum_{i<j}^{M}\delta_{x_i,x_j}\delta_{\alpha_i,-\alpha_j}\Psi^{\{\alpha\}}(x_1,\ldots,x_M)\\
&\quad + \sum_{j=1}^{M}\sum_{\beta_j=\uparrow,\downarrow}[\delta_{x_j,1}\vec{h}_1\cdot\vec{\sigma}_{\alpha_j,\beta_j}+\delta_{x_j,N}\vec{h}_N\cdot\vec{\sigma}_{\alpha_j,\beta_j}]\Psi^{\{\alpha\}_j}(x_1,\ldots,x_M)\\
&= E\,\Psi^{\{\alpha\}}(x_1,\ldots,x_M),
\end{aligned} \tag{2.4}$$

where $\{\alpha\}_j$ means α_j is replaced by β_j in the set $\{\alpha\}$ and $\vec{\sigma} = (\sigma^x,\sigma^y,\sigma^z)$ with σ^x, σ^y and σ^z being the Pauli matrices. The wave function takes the following Bethe ansatz form [9]:

$$\Psi^{\{\alpha\}}(x_1,\ldots,x_M) = \sum_{P,Q,r} A_P^{\{\alpha\},r}(Q)\exp\left[i\sum_{j=1}^{M} r_{P_j}k_{P_j}x_{Q_j}\right]\theta(x_{Q_1}<x_{Q_2}<\cdots<x_{Q_M}), \tag{2.5}$$

where $P = (P_1,\ldots,P_M)$ and $Q = (Q_1,\ldots,Q_M)$ are the permutations of $(1,\ldots,M)$; $r = (r_1,\ldots,r_M)$ with $r_j = \pm$ and $\theta(x_1<\cdots<x_M)$ is the generalized step function. For all $x_j \neq 1, N$ and $x_j \neq x_l$ case, (2.4) is automatically satisfied and the corresponding eigenvalue is

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

For two electrons occupy the same site case, we should consider the continuity of the wave function $\Psi^{\{\alpha\}}(x_1, \ldots, x_M)$. Considering the sector I: $x_{Q_1} < x_{Q_2} < \cdots < x_{Q_j} < x_{Q_{j+1}} < \cdots < x_{Q_M}$ and the sector II: $x_{Q_1} < x_{Q_2} < \cdots < x_{Q_{j+1}} < x_{Q_j} < \cdots < x_{Q_M}$, when $x_{Q_j} = x_{Q_{j+1}} = x$, the continuity of the wave function $\Psi^{\{\alpha\}}(x_1, \ldots, x_M)$ demands

$$\Psi_{\mathrm{I}}^{\{\alpha\}}(\ldots, x, x, \ldots) = \Psi_{\mathrm{II}}^{\{\alpha\}}(\ldots, x, x, \ldots). \tag{2.7}$$

For convenience, we omit the superscript $\{\alpha\}$ and treat $A_P^r(Q)$ as a column vector in the spin space. Then the continuity condition (2.7) of the wave function implies

$$A_P^r(Q) + A_{P'}^{r'}(Q) = A_P^r(Q') + A_{P'}^{r'}(Q'), \tag{2.8}$$

where $Q' = (\ldots, Q_{j+1}, Q_j, \ldots)$, $P' = (\ldots, P_{j+1}, P_j, \ldots)$ and $r' = (\ldots, r_{j+1}, r_j, \ldots)$. For $x_{Q_j} = x_{Q_{j+1}} \neq 1, N$, the Schrödinger equation (2.4) gives

$$\begin{aligned} &-t\big[A_P^r(Q')e^{ir_{P_{j+1}}k_{P_{j+1}}} + A_{P'}^{r'}(Q')e^{ir_{P_j}k_{P_j}} + A_P^r(Q)e^{-ir_{P_j}k_{P_j}} + A_{P'}^{r'}(Q)e^{-ir_{P_{j+1}}k_{P_{j+1}}} \\ &\quad + A_P^r(Q)e^{ir_{P_{j+1}}k_{P_{j+1}}} + A_{P'}^{r'}(Q)e^{ir_{P_j}k_{P_j}} + A_P^r(Q')e^{-ir_{P_j}k_{P_j}} + A_{P'}^{r'}(Q')e^{-ir_{P_{j+1}}k_{P_{j+1}}}\big] \\ &\quad + U\big[A_P^r(Q) + A_{P'}^{r'}(Q)\big] = -2t[\cos k_{P_j} + \cos k_{P_{j+1}}]\big[A_P^r(Q) + A_{P'}^{r'}(Q)\big]. \end{aligned} \tag{2.9}$$

Substituting (2.8) into (2.9), we have

$$\begin{aligned} &\big[\sin(r_{p_j}k_{p_j}) - \sin(r_{p_{j+1}}k_{p_{j+1}})\big]A_P^r(Q) - i\frac{U}{2t}A_P^r(Q') \\ &\quad = \left[\sin(r_{p_j}k_{p_j}) - \sin(r_{p_{j+1}}k_{p_{j+1}}) + i\frac{U}{2t}\right]A_{P'}^{r'}(Q'). \end{aligned} \tag{2.10}$$

Now, we define the coordinate permutation operator $\bar{P}_{i,j}$,

$$\bar{P}_{i,j}A_P^r(\ldots, x_{Q_i}, \ldots, x_{Q_j}, \ldots) = A_P^r(\ldots, x_{Q_j}, \ldots, x_{Q_i}, \ldots). \tag{2.11}$$

Due to the fact that the wave function of fermion is completely antisymmetric under exchanging both the coordinates and spins of two particles, if we denote $P_{i,j}$ as the spin permutation operator, we have

$$P_{i,j}\bar{P}_{i,j} = -1, \qquad P_{i,j}^2 = \bar{P}_{i,j}^2 = 1. \tag{2.12}$$

Thus, we have the following relation:

$$-P_{j,j+1}A_P^r(Q) = A_P^r(Q'). \tag{2.13}$$

Substituting this relation into (2.10), we readily have

$$A_P^r(Q) = S_{P_j,P_{j+1}}(r_{P_j}k_{P_j}, r_{P_{j+1}}k_{P_{j+1}})A_{P'}^{r'}(Q'), \tag{2.14}$$

with the S-matrix given by

$$S_{j,l}(k_j, k_l) = \frac{\sin k_j - \sin k_l - i\frac{U}{2t}P_{j,l}}{\sin k_j - \sin k_l - i\frac{U}{2t}}. \tag{2.15}$$

Now let us turn to the case of $x_{Q_1} = 1$, $x_{Q_i} \neq x_{Q_j}$ $(i \neq j)$ and $x_{Q_M} \neq N$. In this case, the eigenvalue equation (2.4) becomes

$$-t\Psi^{\{\alpha\}}(2,\ldots) + \sum_{\beta_1} \vec{h}_1 \cdot \vec{\sigma}_{\alpha_1,\beta_1} \Psi^{(\beta_1,\ldots)}(1,\ldots) = -2t\cos k_{P_1} \Psi^{\{\alpha\}}(1,\ldots). \tag{2.16}$$

This induces

$$\sum_{\beta_1} \vec{h}_1 \cdot \vec{\sigma}_{\alpha_1,\beta_1} \Psi^{(\beta_1,\ldots)}(1,\ldots) = -t\Psi^{\{\alpha\}}(0,\ldots), \tag{2.17}$$

which gives

$$\begin{aligned} A_P^{(+,\ldots)}(Q) &= -\big[t + \vec{h}_1 \cdot \vec{\sigma}_1 e^{ik_{P_1}}\big]^{-1}\big[t + \vec{h}_1 \cdot \vec{\sigma}_1 e^{-ik_{P_1}}\big] A_P^{(-,\ldots)}(Q) \\ &\stackrel{\text{def}}{=} \bar{K}_1^+(k_{P_1}) A_P^{(-,\ldots)}(Q). \end{aligned} \tag{2.18}$$

With the help of the identity

$$(\vec{h}_1 \cdot \vec{\sigma})^2 = \vec{h}_1^2,$$

we have

$$\bar{K}_j^+(k) = -\frac{t^2 - \vec{h}_1^2 - 2it\sin k\, \vec{h}_1 \cdot \vec{\sigma}_j}{t^2 - \vec{h}_1^2 e^{2ik}}. \tag{2.19}$$

Similarly, for the case of $x_{Q_M} = N$, $x_{Q_i} \neq x_{Q_j}$ $(i \neq j)$ and $x_{Q_1} \neq 1$, we have

$$-t\Psi^{\{\alpha\}}(\ldots, N-1) + \sum_{\beta_M} \vec{h}_N \cdot \vec{\sigma}_{\alpha_M,\beta_M} \Psi^{(\ldots,\beta_M)}(\ldots,N) = -2t\cos k_{P_M} \Psi^{\{\alpha\}}(\ldots,N), \tag{2.20}$$

namely,

$$\sum_{\beta_M} \vec{h}_N \cdot \vec{\sigma}_{\alpha_M,\beta_M} \Psi^{(\ldots,\beta_M)}(\ldots,N) = -t\Psi^{\{\alpha\}}(\ldots,N+1), \tag{2.21}$$

which induces

$$\begin{aligned} e^{-2ik_{P_M}N} A_P^{(\ldots,-)}(Q) &= -\big[te^{-ik_{P_M}} + \vec{h}_N \cdot \vec{\sigma}_M\big]^{-1}\big[te^{ik_{P_M}} + \vec{h}_N \cdot \vec{\sigma}_M\big] A_P^{(\ldots,+)}(Q) \\ &\stackrel{\text{def}}{=} \bar{K}_M^-(k_{P_M}) A_P^{(\ldots,+)}(Q), \end{aligned} \tag{2.22}$$

with

$$\bar{K}_j^-(k) = -\frac{t^2 - \vec{h}_N^2 - 2it\sin k\, \vec{h}_N \cdot \vec{\sigma}_j}{t^2 e^{-2ik} - \vec{h}_N^2}. \tag{2.23}$$

When $x_{Q_1} = x_{Q_2} = 1$ or $x_{Q_{M-1}} = x_{Q_M} = N$, the situation becomes a little bit subtle. We have to check the self-consistence of the ansatz. For the case of $x_{Q_1} = x_{Q_2} = 1$, $x_{Q_i} \neq x_{Q_j}$ $(i \neq j$ and $i, j \neq 1)$ and $x_{Q_M} \neq N$, the eigenvalue equation (2.4) becomes

$$\begin{aligned} &-t\big[\Psi^{\{\alpha\}}(2,1,\ldots) + \Psi^{\{\alpha\}}(1,2,\ldots)\big] + U\Psi^{\{\alpha\}}(1,1,\ldots) \\ &\quad + \sum_{\beta_1,\beta_2} [\vec{h}_1 \cdot \vec{\sigma}_{\alpha_1,\beta_1} + \vec{h}_1 \cdot \vec{\sigma}_{\alpha_2,\beta_2}] \Psi^{(\beta_1,\beta_2,\ldots)}(1,1,\ldots) \\ &= -2t[\cos k_{P_1} + \cos k_{P_2}] \Psi^{\{\alpha\}}(1,1,\ldots). \end{aligned} \tag{2.24}$$

And in this case, the S-matrix makes the following equation hold:

$$\begin{aligned} &-t\big[\Psi^{\{\alpha\}}(2,1,\ldots)+\Psi^{\{\alpha\}}(0,1,\ldots)+\Psi^{\{\alpha\}}(1,2,\ldots) \\ &\quad +\Psi^{\{\alpha\}}(1,0,\ldots)\big]+U\Psi^{\{\alpha\}}(1,1,\ldots) \\ &= -2t[\cos k_{P_1}+\cos k_{P_2}]\Psi^{\{\alpha\}}(1,1,\ldots). \end{aligned} \tag{2.25}$$

Combining Eq. (2.24) and Eq. (2.25), we have the following relation need to be confirmed:

$$-t\big[\Psi^{\{\alpha\}}(0,1,\ldots)+\Psi^{\{\alpha\}}(1,0,\ldots)\big]=\sum_{\beta_1,\beta_2}[\vec{h}_1\cdot\vec{\sigma}_{\alpha_1,\beta_1}+\vec{h}_1\cdot\vec{\sigma}_{\alpha_2,\beta_2}]\Psi^{(\beta_1,\beta_2,\ldots)}(1,1,\ldots). \tag{2.26}$$

For the case of $x_{Q_1}=1$, $x_{Q_i}\neq x_{Q_j}$ $(i\neq j)$ and $x_{Q_M}\neq N$, we have the relation (2.17). For $x_{Q_2}=1$, $x_{Q_i}\neq x_{Q_j}(i\neq j)$ and $x_{Q_M}\neq N$, similarly, we have

$$\sum_{\beta_2}\vec{h}_1\cdot\vec{\sigma}_{\alpha_2,\beta_2}\Psi^{(\alpha_1,\beta_2,\ldots)}(1,1,\ldots)=-t\Psi^{\{\alpha\}}(1,0,\ldots). \tag{2.27}$$

Obviously (2.17) and (2.27) make (2.26) hold. With the same procedure we can demonstrate that the ansatz is also satisfied when two electrons both occupy the site N.

Now let us consider the following process. The j-th particle moves from the l-th site to the left end by scattering with all the other particles to their left, and then is reflected by the left boundary. After scattering with all the other particles, it is reflected by the right boundary and then moves back to its original position. This process can be described by the following relations:

$$\begin{aligned} A^{(\ldots,+,\ldots)} &= S_{j-1,j}(k_{j-1},k_j)S_{j-2,j}(k_{j-2},k_j)\cdots S_{1,j}(k_1,k_j)A^{(+,\ldots)}, \\ A^{(+,\ldots)} &= \bar{K}_j^{+}(k_j)\,A^{(-,\ldots)}, \\ A^{(-,\ldots)} &= S_{j,1}(-k_j,k_1)\cdots S_{j,j-1}(-k_j,k_{j-1}) \\ &\quad\times S_{j,j+1}(-k_j,k_{j+1})\cdots S_{j,M}(-k_j,k_M)A^{(\ldots,-)}, \\ A^{(\ldots,-)} &= e^{2ik_jN}\bar{K}_j^{-}(k_j)\,A^{(\ldots,+)}, \\ A^{(\ldots,+)} &= S_{M,j}(k_M,k_j)\cdots S_{j+1,j}(k_{j+1},k_j)A^{(\ldots,+,\ldots)}. \end{aligned}$$

Consequently, this gives rise to the following eigenvalue problem:

$$\bar{\tau}(k_j)A^{(\ldots,+,\ldots)}=e^{-2ik_jN}A^{(\ldots,+,\ldots)}, \tag{2.28}$$

with the resulting operators

$$\begin{aligned} \bar{\tau}(k_j) &= S_{j-1,j}(k_{j-1},k_j)\cdots S_{1,j}(k_1,k_j)\bar{K}_j^{+}(k_j)S_{j,1}(-k_j,k_1)\cdots S_{j,j-1}(-k_j,k_{j-1}) \\ &\quad\times S_{j,j+1}(-k_j,k_{j+1})\cdots S_{j,M}(-k_j,k_M)\bar{K}_j^{-}(k_j) \\ &\quad\times S_{M,j}(k_M,k_j)\cdots S_{j+1,j}(k_{j+1},k_j). \end{aligned} \tag{2.29}$$

Let $\mathbf{V}$ denotes a two-dimensional linear space. Throughout the paper we adopt the standard notations: for any matrix $A\in \mathrm{End}(\mathbf{V})$, A_j is an embedding operator in the tensor space $\mathbf{V}\otimes\mathbf{V}\otimes\cdots$, which acts as A on the j-th space and as identity on the other factor spaces; $R_{ij}(u)$ is an embedding operator of R-matrix in the tensor space, which acts as identity on the factor spaces except for the i-th and j-th ones.

In the next section we shall show that $\bar{\tau}(k_j)$ is proportional to the transfer matrix of the inhomogeneous XXX spin chain with arbitrary boundary fields and thus the eigenvalue problem (2.28) can be further solved by the off-diagonal Bethe ansatz method.

3. Off-diagonal Bethe ansatz

Before going further, let us introduce the following R-matrix and K-matrices:

$$R_{0,j}(u) = u + \eta P_{0,j}, \tag{3.1}$$

$$K_0^-(u) = p + u \vec{h}_N \cdot \vec{\sigma}_0, \tag{3.2}$$

$$K_0^+(u) = q - (u+\eta) \vec{h}_1 \cdot \vec{\sigma}_0, \tag{3.3}$$

where

$$\eta = -i\frac{U}{2t}, \qquad p = i\frac{\vec{h}_N^2 - t^2}{2t}, \qquad q = i\frac{t^2 - \vec{h}_1^2}{2t}.$$

The R-matrix possesses the following properties:

$$\text{Initial condition:} \quad R_{1,2}(0) = \eta P_{1,2}, \tag{3.4}$$

$$\text{Unitarity relation:} \quad R_{1,2}(u) R_{1,2}(-u) = -(u+\eta)(u-\eta)\,\mathrm{id}, \tag{3.5}$$

$$\text{Crossing relation:} \quad R_{12}(u) = V_1 R_{12}^{t_2}(-u-\eta) V_1, \qquad V = -i\sigma^y. \tag{3.6}$$

The following Yang–Baxter equation, the reflection equation and its dual also hold:

$$R_{0,0'}(u-v) R_{0,1}(u) R_{0',1}(v) = R_{0',1}(v) R_{0,1}(u) R_{0,0'}(u-v), \tag{3.7}$$

$$R_{0,0'}(u-v) K_0^-(u) R_{0,0'}(u+v) K_{0'}^-(v) = K_{0'}^-(v) R_{0,0'}(u+v) K_0^-(u) R_{0,0'}(u-v), \tag{3.8}$$

$$\begin{aligned} &R_{0,0'}(v - K_0^+(u) R_{0,0'}(-u-v-2\eta) K_{0'}^+(v) \\ &\quad = K_{0'}^+(v) R_{0,0'}(-u-v-\eta) K_0^+(u) R_{0,0'}(v-u). \end{aligned} \tag{3.9}$$

Now let us define the inhomogeneous double-row monodromy matrix[1] [19,21],

$$\begin{aligned} T_0(u) = {} & R_{0,1}(u - \sin k_1) \cdots R_{0,M}(u - \sin k_M) K_0^-(u) \\ & \times R_{M,0}(u + \sin k_M) \cdots R_{1,0}(u + \sin k_1), \end{aligned} \tag{3.10}$$

and the transfer matrix $\tau(u)$,

$$\tau(u) = \mathrm{tr}_0\big\{K_0^+(u) T_0(u)\big\}. \tag{3.11}$$

From the Yang–Baxter equation and the reflection equation and its dual one may derive [19]

$$R_{0,0'}(u-v) T_0(u) R_{0,0'}(u+v) T_{0'}(v) = T_{0'}(v) R_{0,0'}(u+v) T_0(u) R_{0,0'}(u-v), \tag{3.12}$$

and the transfer matrices with different spectrum parameters commute with each other,

$$\big[\tau(u), \tau(v)\big] = 0. \tag{3.13}$$

Putting $u = -\sin k_j$, we readily have

[1] In order to compare with the operators (2.29), we choose the inhomogeneous parameters $\theta_j = \sin k_j$.

$$\begin{aligned}\tau(-\sin k_j) = {} & R_{j-1,j}(-\sin k_j + \sin k_{j-1}) \cdots R_{1,j}(-\sin k_j + \sin k_1) \\ & \times \mathrm{tr}_0\big\{K_0^+(-\sin k_j) R_{0,j}(-2\sin k_j) R_{0,j}(0)\big\} \\ & \times R_{j,1}(-\sin k_j - \sin k_1) \cdots R_{j,j-1}(-\sin k_j - \sin k_{j-1}) \\ & \times R_{j,j+1}(-\sin k_j - \sin k_{j+1}) \cdots R_{j,M}(-\sin k_j - \sin k_M) \\ & \times K_j^-(-\sin k_j) R_{M,j}(-\sin k_j + \sin k_M) \cdots R_{j+1,j}(-\sin k_j + \sin k_{j+1}).\end{aligned} \tag{3.14}$$

Noticing that

$$S_{j,l}(k_j, k_l) = \frac{R_{j,l}(\sin k_j - \sin k_l)}{\sin k_j - \sin k_l + \eta}, \tag{3.15}$$

$$S_{j,l}(-k_j, k_l) = \frac{R_{j,l}(-\sin k_j - \sin k_l)}{-\sin k_j - \sin k_l + \eta}, \tag{3.16}$$

$$\bar{K}_j^-(k_j) = \frac{2it\, K_j^-(-\sin k_j)}{\vec{h}_N^2 - t^2 e^{-2ik_j}}, \tag{3.17}$$

$$\bar{K}_j^+(k_j) = \frac{\mathrm{tr}_0\{it\, K_0^+(-\sin k_j) R_{0,j}(-2\sin k_j) P_{0,j}\}}{(\sin k_j - \eta)(\vec{h}_1^2 e^{2ik_j} - t^2)}, \tag{3.18}$$

we have the following important identification between the operators $\{\bar{\tau}(k_j)\}$ (2.29) appeared in the eigenvalue problem of the open-boundary Hubbard model and the transfer matrix of the open XXX spin chain with boundary fields:

$$\begin{aligned}\bar{\tau}(k_j) = {} & \prod_{l\neq j}^{M} (\sin k_j - \sin k_l - \eta)^{-1} (\sin k_j + \sin k_l - \eta)^{-1} \\ & \times \frac{-2t^2\, \tau(-\sin k_j)}{\eta(\sin k_j - \eta)(t^2 - \vec{h}_1^2 e^{2ik_j})(t^2 e^{-2ik_j} - \vec{h}_N^2)}.\end{aligned} \tag{3.19}$$

The eigenvalue problem (2.28) is thus equivalent to that of diagonalizing the transfer matrix of the inhomogeneous open XXX chain model with boundary fields. Here we naturally have the "inhomogeneous" parameters $\theta_j = \sin k_j$ and the crossing parameter $\eta = -i\frac{U}{2t}$. Thanks to the works [22–24], the transfer matrix (3.11) of the open XXX chain with arbitrary boundary fields which is specified by the K-matrices $K^{\pm}(u)$ (3.2) and (3.3) can be exactly diagonalized by off-diagonal Bethe ansatz method. In the following, we shall use the method in [24] to the eigenvalue problem (2.28) of the Hubbard model with arbitrary boundary fields.

For this purpose, we introduce some functions at first:

$$A(u) = \prod_{l=1}^{M} (u - \sin k_l + \eta)(u + \sin k_l + \eta), \tag{3.20}$$

$$a(u) = \frac{2u + 2\eta}{2u + \eta}\big(p + u\, \mathrm{sgn}(\vec{h}_1 \cdot \vec{h}_N)|\vec{h}_N|\big)\big(q - u\, |\vec{h}_1|\big) A(u), \tag{3.21}$$

$$d(u) = a(-u - \eta), \tag{3.22}$$

$$c = 2\big(\mathrm{sgn}(\vec{h}_1 \cdot \vec{h}_N)|\vec{h}_1||\vec{h}_N| - \vec{h}_1 \cdot \vec{h}_N\big). \tag{3.23}$$

3.1. Even M case

Following [24], we construct the following ansatz of the eigenvalue of the transfer matrix $\tau(u)$ for an even M:

$$\Lambda(u)=a(u)\frac{Q_1(u-\eta)}{Q_2(u)}+d(u)\frac{Q_2(u+\eta)}{Q_1(u)}+c\,u(u+\eta)\frac{A(u)A(-u-\eta)}{Q_1(u)Q_2(u)}, \tag{3.24}$$

in which the functions $Q_1(u)$ and $Q_2(u)$ are parameterized by M different from each other parameters $\{\mu_j \mid j=1,\dots,M\}$ for a generic non-vanishing c as follows:

$$Q_1(u)=\prod_{j=1}^{M}(u-\mu_j), \tag{3.25}$$

$$Q_2(u)=\prod_{j=1}^{M}(u+\mu_j+\eta)=Q_1(-u-\eta). \tag{3.26}$$

It has been shown [24] that $\Lambda(u)$ becomes the eigenvalue of the transfer matrix $\tau(u)$ given by (3.11) if the M parameters $\{\mu_j \mid j=1,\dots,M\}$ satisfies the following Bethe ansatz equations:

$$\frac{c\,(\mu_j+\eta)(\mu_j+\frac{\eta}{2})}{(p-(\mu_j+\eta)\,\mathrm{sgn}(\vec{h}_1\cdot\vec{h}_N)|\vec{h}_N|)(q+(\mu_j+\eta)|\vec{h}_1|)}$$
$$=-\prod_{l=1}^{M}\frac{(\mu_j+\mu_l+\eta)(\mu_j+\mu_l+2\eta)}{(\mu_j-\sin k_l+\eta)(\mu_j+\sin k_l+\eta)},\qquad j=1,\dots,M, \tag{3.27}$$

where the parameter c is expressed in terms of the boundary fields (3.23). Numerical checks of the completeness of the above solutions for small size of M (the results for the odd M see the next subsection) was given in [25,26] (see also [27]). A beautiful expression for the corresponding eigenvectors was proposed recently in [28].

Based on the expressions (3.24) of $\Lambda(u)$ for the eigenvalue of the transfer matrix (3.11) and the relation (3.19) between the operator $\bar{\tau}(k_j)$ and the transfer matrix at special point $\tau(-\sin k_j)$, the eigenvalue problem (2.28) gives rise to the following constraints on the quasi-momentum $\{k_j\}$:

$$e^{-2ik_jN}=\prod_{l\neq j}^{M}(\sin k_j-\sin k_l-\eta)^{-1}(\sin k_j+\sin k_l-\eta)^{-1}$$
$$\times\frac{-2t^2\Lambda(-\sin k_j)}{\eta(\sin k_j-\eta)(t^2-\vec{h}_1^2e^{2ik_j})(t^2e^{-2ik_j}-\vec{h}_N^2)}. \tag{3.28}$$

Noticing that $d(-\sin k_j)=A(\sin k_j-\eta)=0$, the above Bethe ansatz equations become

$$\frac{4t^2(p-\sin k_j\,\mathrm{sgn}(\vec{h}_1\cdot\vec{h}_N)|\vec{h}_N|)(q+\sin k_j\,|\vec{h}_1|)}{(t^2-\vec{h}_1^2e^{2ik_j})(t^2e^{-2ik_j}-\vec{h}_N^2)}=e^{-2ik_jN}\prod_{l=1}^{M}\frac{(\sin k_j-\mu_l-\eta)}{(\sin k_j+\mu_l+\eta)},$$
$$j=1,\dots,M. \tag{3.29}$$

Then from the solutions of the Bethe ansatz equations (3.27) and (3.29), one can reconstruct the exact wave functions (2.5) with even number of electrons for the Hubbard model with boundary fields, the corresponding eigenvalues are given by (2.6).

3.2. Odd M case

Following [24], we construct the following ansatz of the eigenvalue of the transfer matrix $\tau(u)$ for an odd M:

$$\Lambda(u) = a(u)\frac{Q_1(u-\eta)}{Q_2(u)} + d(u)\frac{Q_2(u+\eta)}{Q_1(u)} + c\,u^2(u+\eta)^2\frac{A(u)A(-u-\eta)}{Q_1(u)Q_2(u)}, \tag{3.30}$$

where the functions $a(u)$, $d(u)$ and $A(u)$ and the parameter c are given by (3.20)–(3.23) respectively. The functions $Q_1(u)$ and $Q_2(u)$ are some functions parameterized by $M+1$ different from each other parameters $\{\mu_j \mid j = 1, \ldots, M+1\}$ for a generic non-vanishing c as follows:

$$Q_1(u) = \prod_{j=1}^{M+1}(u-\mu_j), \tag{3.31}$$

$$Q_2(u) = \prod_{j=1}^{M+1}(u+\mu_j+\eta) = Q_1(-u-\eta). \tag{3.32}$$

Keeping the expression (3.30) of the function $\Lambda(u)$ in mind, we find that the M quasi-momentum $\{k_j\}$ and the $M+1$ parameters $\{\mu_j \mid j = 1, \ldots, M+1\}$ need to satisfy the following Bethe ansatz equations:

$$\frac{4t^2(p - \sin k_j\,\mathrm{sgn}(\vec{h}_1\cdot\vec{h}_N)|\vec{h}_N|)(q + \sin k_j\,|\vec{h}_1|)}{(t^2 - \vec{h}_1^2 e^{2ik_j})(t^2 e^{-2ik_j} - \vec{h}_N^2)} = e^{-2ik_jN}\prod_{l=1}^{M+1}\frac{(\sin k_j - \mu_l - \eta)}{(\sin k_j + \mu_l + \eta)},$$
$$j = 1, \ldots, M, \tag{3.33}$$

$$\frac{-c\,\mu_j(\mu_j+\frac{\eta}{2})(\mu_j+\eta)^2}{(p-(\mu_j+\eta)\,\mathrm{sgn}(\vec{h}_1\cdot\vec{h}_N)|\vec{h}_N|)(q+(\mu_j+\eta)|\vec{h}_1|)} \times \prod_{l=1}^{M}(\mu_j - \sin k_l + \eta)(\mu_j + \sin k_l + \eta)$$
$$= \prod_{l=1}^{M+1}(\mu_j+\mu_l+\eta)(\mu_j+\mu_l+2\eta), \quad j = 1, \ldots, M+1. \tag{3.34}$$

From the solutions of the Bethe ansatz equations (3.33) and (3.34), one can reconstruct the exact wave functions (2.5) with odd number of electrons for the Hubbard model with boundary fields, the corresponding eigenvalues are given by (2.6).

4. Reduction to the parallel boundary case

When the two boundary fields $\vec{h}_1$ and $\vec{h}_N$ are parallel or anti-parallel, the $U(1)$ symmetry in the spin sector is recovered, and the associated open XXX spin chain is specified by two diagonal K-matrices. In our method the corresponding parameter c given by (3.23) is vanishing. The resulting T–Q ansatz of the eigenvalue of the transfer matrix of the associated spin chain reduces to the usual form no matter M is even or odd [24]:

$$\Lambda(u) = a(u)\frac{Q(u-\eta)}{Q(u)} + d(u)\frac{Q(u+\eta)}{Q(u)}, \tag{4.1}$$

where the functions $Q(u)$ are parameterized by m different from each other Bethe roots $\{\lambda_j \mid j=1,\ldots,m\}$ with discrete $m=0,\ldots,M$ as follows:

$$Q(u)=\prod_{l=1}^{m}(u-\lambda_l)(u+\lambda_l+\eta)=Q(-u-\eta). \tag{4.2}$$

Here the discrete number m is the consequence of the $U(1)$ symmetry reservation in the case that the two boundary fields $\vec{h}_1$ and $\vec{h}_N$ are parallel or anti-parallel. These m parameters $\{\lambda_j\}$ and M quasi-momentum $\{k_j\}$ satisfy the following Bethe ansatz equations:

$$\frac{4t^2(p-\sin k_j|\vec{h}_N|)(q+\sin k_j|\vec{h}_1|)}{(t^2-\vec{h}_1^2e^{2ik_j})(t^2e^{-2ik_j}-\vec{h}_N^2)}=e^{-2ik_jN}\prod_{l=1}^{m}\frac{(\sin k_j+\lambda_l)(\sin k_j-\lambda_l-\eta)}{(\sin k_j-\lambda_l)(\sin k_j+\lambda_l+\eta)},$$
$$j=1,\ldots,M, \tag{4.3}$$

$$\frac{\lambda_j(p-(\lambda_j+\eta)|\vec{h}_N|)(q+(\lambda_j+\eta)|\vec{h}_1|)}{(\lambda_j+\eta)(p+\lambda_j|\vec{h}_N|)(q-\lambda_j|\vec{h}_1|)}\prod_{l=1}^{M}\frac{(\lambda_j+\sin k_l)(\lambda_j-\sin k_l)}{(\lambda_j-\sin k_l+\eta)(\lambda_j+\sin k_l+\eta)}$$
$$=-\prod_{l=1}^{m}\frac{(\lambda_j-\lambda_l-\eta)(\lambda_j+\lambda_l)}{(\lambda_j-\lambda_l+\eta)(\lambda_j+\lambda_l+2\eta)},\quad j=1,\ldots,m. \tag{4.4}$$

From the solutions of the Bethe ansatz equations (4.3) and (4.4), one can reconstruct the exact wave functions (2.5) for the Hubbard model with parallel or anti-parallel boundary fields, the corresponding eigenvalues are given by (2.6).

5. Conclusion

The one-dimensional Hubbard model with arbitrary boundary magnetic fields described by the Hamiltonian (1.1) is studied by combining the coordinate Bethe ansatz and off-diagonal Bethe ansatz methods. With the coordinate Bethe ansatz, eigen-functions of the Hamiltonian of the model are given in terms of some quasi-momentum $\{k_j\}$ as (2.5). The constraints (2.28) on these quasi-momentum is transformed into the eigenvalues problem of the resulting transfer matrix of the associated open XXX spin chain with arbitrary boundary fields. The second eigenvalue problem is then solved via the off-diagonal Bethe ansatz method. The corresponding Bethe ansatz equations (3.27) and (3.29) for the even number of electrons case, (3.33) and (3.34) for the odd number of electrons are constructed respectively when two boundary fields are unparallel, which corresponds to the case of the $U(1)$ symmetry in the spin sector being broken. When the two boundary fields $\vec{h}_1$ and $\vec{h}_N$ are parallel or anti-parallel, the $U(1)$ symmetry in spin sector is recovered, the resulting Bethe ansatz equations become (4.3) and (4.4) which are labeled by a discrete number $m=0,\ldots,M$.

Acknowledgements

Y. Wang would like to thank X.W. Guan for fruitful discussions. The financial support from the National Natural Science Foundation of China (Grant Nos. 11174335, 11075126, 11031005, 11375141, 11374334), the National Program for Basic Research of MOST (973 project under grant No. 2011CB921700), the State Education Ministry of China (Grant No. 20116101110017) and BCMIIS are gratefully acknowledged.

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