Integrable Boundary Conditions for the One-Dimensional Hubbard Model

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Abstract

We discuss the integrable boundary conditions for the one-dimensional (1D) Hubbard Model in the framework of the Quantum Inverse Scattering Method (QISM). We use the fermionic $R$-matrix proposed by Olmedilla et al. to treat the twisted periodic boundary condition and the open boundary condition. We determine the most general form of the integrable twisted periodic boundary condition by considering the symmetry matrix of the fermionic $R$-matrix. To find the integrable open boundary condition, we shall solve the graded reflection equation, and find there are two diagonal solutions, which correspond to a) the boundary chemical potential and b) the boundary magnetic field. Non-diagonal solutions are obtained using the symmetry matrix of the fermionic $R$-matrix and the covariance property of the graded reflection equation. They can be interpreted as the $SO(4)$ rotations of the diagonal solutions.

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§1. Introduction

The one-dimensional (1D) Hubbard model is one of the most important solvable models in condensed matter physics. The ground state energy of the 1D Hubbard model

\[ \hat{H} = - \sum_{m=1}^{N} \sum_{s=\uparrow,\downarrow} (c_{ms}^{\dagger} c_{m+1s} + c_{m+1s}^{\dagger} c_{ms}) + U \sum_{m=1}^{N} (n_{m\uparrow} - \frac{1}{2})(n_{m\downarrow} - \frac{1}{2}), \]  

(1.1)

with periodic boundary condition

\[ c_{N+1s}^{\dagger} = c_{1s}^{\dagger}, \quad c_{N+1s} = c_{1s} \quad (s=\uparrow,\downarrow), \]  

(1.2)

was obtained by Lieb and Wu \[1\] by means of the coordinate Bethe ansatz method. Here \( c_{ms}^{\dagger} \) and \( c_{ms} \) are the fermionic creation and annihilation operators with spin \( s(=\uparrow,\downarrow) \) at site \( m(=1,2,\ldots,N) \), and \( n_{ms} \) is the number density operator

\[ n_{ms} = c_{ms}^{\dagger} c_{ms}. \]  

(1.3)

The parameter \( U \) is the coupling constant describing the Coulomb interaction. The bulk properties of the 1D Hubbard model have been clarified by analyzing the associated Bethe ansatz equations \[2\].

As is well known, the Hamiltonian (1.1) enjoys two \( SU(2) \) symmetries \[3–7\], which are the spin-\( SU(2) \) generated by

\[ S^{+} = \sum_{m=1}^{N} c_{m\uparrow}^{\dagger} c_{m\downarrow}, \quad S^{-} = \sum_{m=1}^{N} c_{m\downarrow}^{\dagger} c_{m\uparrow}, \quad S^{z} = \frac{1}{2} \sum_{m=1}^{N} (n_{m\uparrow} - n_{m\downarrow}), \]  

(1.4)

and the charge-\( SU(2) \) generated by

\[ \eta^{+} = \sum_{m=1}^{N} (-1)^{m} c_{m\uparrow}^{\dagger} c_{m\uparrow}, \quad \eta^{-} = \sum_{m=1}^{N} (-1)^{m} c_{m\downarrow} c_{m\downarrow}, \quad \eta^{z} = \frac{1}{2} \sum_{m=1}^{N} (n_{m\uparrow} + n_{m\downarrow} - 1). \]  

(1.5)

For the consistency of the definition of the charge-\( SU(2) \), it is necessary to assume that the number of the lattice sites \( N \) is even. The spin-\( SU(2) \) and the charge-\( SU(2) \) are connected through the partial particle-hole transformation

\[ c_{m\uparrow} \rightarrow c_{m\uparrow}, \quad c_{m\downarrow} \rightarrow (-1)^{m} c_{m\downarrow}, \quad U \rightarrow -U. \]  

(1.6)

Since a constraint

\[ S^{z} + \eta^{z} = \text{integer} \]  

(1.7)

holds, the exact symmetry of the Hamiltonian (1.1) is \( SO(4) = [SU(2) \times SU(2)]/\mathbb{Z}_2 \). The \( SO(4) \) symmetry may be the most fundamental property of the 1D Hubbard model that characterizes the various physical features of the model. For example, it was proved by Essler et al. that the Bethe ansatz states of the 1D Hubbard model are incomplete and have to be complemented by the \( SO(4) \) symmetry \[8–10\]. Essler and Korepin \[11, 12\] showed that the elementary excitations of the half-filled band constitute the multiplets of \( SO(4) \).

To discuss the bulk properties of the model, we usually assume the periodic boundary condition (1.2), since the bulk physical quantities do not depend on the boundary condition.
However, when we investigate the surface critical phenomena, or the transport properties, it is necessary to pay attention to the boundary condition.  

The twisted periodic boundary condition for the Hubbard model was discussed by Shastry and Sutherland \[13, 14\]. They have shown that the coordinate Bethe ansatz method is applicable if we generalize the periodic boundary conditions to the twisted periodic boundary condition

\[
\begin{align*}
    c_{N+1\uparrow}^\dagger &= e^{i\phi} c_{1\uparrow}^\dagger, \\
    c_{N+1\downarrow}^\dagger &= e^{i\psi} c_{1\downarrow}^\dagger, \\
    c_{N+1\uparrow} &= e^{-i\phi} c_{1\uparrow}, \\
    c_{N+1\downarrow} &= e^{-i\psi} c_{1\downarrow},
\end{align*}
\]

(1.8)

where the parameters $\phi$ and $\psi$ are twist angles. These changes of the boundary condition affect directly the transport properties such as the stiffness constants \[13, 14\].

Recently the 1D Hubbard model with the open boundary condition has attracted much attention. The corresponding Hamiltonian reads

\[
\hat{H}_{\text{open}} = -\sum_{m=1}^{N-1} \left( c_{m\uparrow}^\dagger c_{m+1\downarrow} + c_{m+1\uparrow}^\dagger c_{m\downarrow} \right) + U \sum_{m=1}^{N} \left( n_{m\uparrow} - \frac{1}{2} \right) \left( n_{m\downarrow} - \frac{1}{2} \right) - p_{\uparrow} \left( n_{1\uparrow} - \frac{1}{2} \right) - p_{\downarrow} \left( n_{1\downarrow} - \frac{1}{2} \right) - p_{N\uparrow} \left( n_{N\uparrow} - \frac{1}{2} \right) - p_{N\downarrow} \left( n_{N\downarrow} - \frac{1}{2} \right),
\]

(1.9)

where $p_{1\uparrow}, p_{N\downarrow} (s = \uparrow, \downarrow)$ are the boundary fields that specify the boundary conditions. In the case of vanishing boundary fields $p_{1\uparrow} = p_{N\downarrow} = 0 (s = \uparrow, \downarrow)$, this model was solved by Schulz \[15\] applying the coordinate Bethe ansatz method. More recently, Asakawa and Suzuki \[16\] extended the solution to the boundary chemical potential case $p_{1\uparrow} = p_{1\downarrow} = p_{N\uparrow} = p_{N\downarrow} = p$. The present authors \[17\] studied the consistency conditions for the Bethe ansatz wave functions and classified the possible forms of the boundary fields. It turned out that the boundary fields can be either of the form a) a boundary chemical potential: $p_{m\uparrow} = p_{m\downarrow} = p_m$, or b) a boundary magnetic field: $p_{m\uparrow} = -p_{m\downarrow} = p_m$, where $m = 1$ or $m = N$.

Since the boundary conditions at the different ends are independent, we have four integrable open boundary conditions \[17\]:

- **Case A.** $p_{1\uparrow} = p_{1\downarrow} = p_1$, $p_{N\uparrow} = p_{N\downarrow} = p_N$.
- **Case B.** $p_{1\uparrow} = -p_{1\downarrow} = p_1$, $p_{N\uparrow} = -p_{N\downarrow} = p_N$.
- **Case C.** $p_{1\uparrow} = -p_{1\downarrow} = p_1$, $p_{N\uparrow} = p_{N\downarrow} = p_N$.
- **Case D.** $p_{1\uparrow} = p_{1\downarrow} = p_1$, $p_{N\uparrow} = -p_{N\downarrow} = p_N$.

(1.10)

The corresponding Bethe ansatz equations were derived \[17, 18\].

The exact integrability of the 1D Hubbard model with periodic boundary condition was established by Shastry \[19–21\] and Olmedilla et al. \[22, 23\]. The Jordan-Wigner transformation

\[
\begin{align*}
    c_{m\uparrow}^\dagger &= (\sigma_1^z \cdots \sigma_{m-1}^z) \sigma_m^- \\
    c_{m\downarrow}^\dagger &= (\sigma_1^z \cdots \sigma_N^z) (\tau_1^z \cdots \tau_{m-1}^z) \tau_m^-,
\end{align*}
\]

(1.11)

changes the fermionic Hamiltonian (1.1) into an equivalent coupled spin model

\[
H = \sum_{m=1}^{N} (\sigma_{m+1}^\dagger \sigma_m^- + \sigma_m^\dagger \sigma_{m+1}^-) + \sum_{m=1}^{N} (\tau_{m+1}^\dagger \tau_m^- + \tau_m^\dagger \tau_{m+1}^-) + \frac{U}{4} \sum_{m=1}^{N} \sigma_m^z \tau_m^z,
\]

(1.12)
where $\sigma$ and $\tau$ are two species of the Pauli matrices commuting among each other, and
\[
\sigma_m^\pm = \frac{1}{2} (\sigma_m^x \pm i \sigma_m^y), \quad \tau_m^\pm = \frac{1}{2} (\tau_m^x \pm i \tau_m^y).
\] (1.13)

Shastry constructed the $L$-operator and the $R$-matrix which satisfy the Yang-Baxter relation, "$RLL = LLR$", for the equivalent coupled spin model (1.12). The present authors proved the Yang-Baxter equation, "$RRR = RRR$", for Shastry’s $R$-matrix [24–26].

It is well known that the Jordan-Wigner transformation (1.11) is not consistent with the periodic boundary condition for the fermion operators (1.2). In fact, the periodic boundary condition for the fermionic operators (1.2) corresponds to a sector dependent twisted boundary condition for the coupled spin model (1.12)
\[
(\prod_{m=1}^{N} \sigma^z_m ) \sigma_{N+1}^\pm = \sigma_1^\pm, \quad (\prod_{m=1}^{N} \tau^z_m ) \tau_{N+1}^\pm = \tau_1^\pm.
\] (1.14)

Hence it is more natural to use the fermionic formulation developed by Olmedilla et al. [22, 23], when we discuss the boundary conditions for the 1D Hubbard model. They proposed the fermionic $L$-operator and the fermionic $R$-matrix which satisfy the graded Yang-Baxter relation. The transfer matrix which corresponds to the fermionic 1D Hubbard model with the periodic boundary condition is constructed by taking the supertrace of the monodromy matrix [22, 23].

In this paper, as a first problem, we shall generalize their results to the case of the twisted periodic boundary condition. We shall find the symmetry matrix of the fermionic $R$-matrix, which is the constant solution of the graded Yang-Baxter relation. It is closely related to the $SO(4)$ symmetry of the Hamiltonian (1.1). The symmetry matrix can be inserted into the transfer matrix without breaking the integrability [27]. We shall show that the periodic boundary condition is twisted by the insertion of the symmetry matrix.

A general method to prove the exact integrability of the model with open boundaries was developed by Sklyanin [27]. Through the Jordan-Wigner transformation, the Hamiltonian (1.9) is transformed into
\[
H_{\text{open}} = \sum_{m=1}^{N-1} \left( \sigma^+_m \sigma^-_{m+1} + \sigma^-_m \sigma^+_m \right) + \sum_{m=1}^{N-1} \left( \tau^+_m \tau^-_{m+1} + \tau^-_m \tau^+_m \right) + \frac{U}{4} \sum_{m=1}^{N} \sigma^z_m \tau^z_m - \frac{p_{1\uparrow}}{2} \sigma^z_1 - \frac{p_{N\uparrow}}{2} \sigma^z_N - \frac{p_{1\downarrow}}{2} \tau^z_1 - \frac{p_{N\downarrow}}{2} \tau^z_N.
\] (1.15)

Zhou [28] applied the Sklyanin’s formalism to investigate the exact integrability of the model (1.13). He formulated the reflection equation in terms of Shastry’s $R$-matrix and found a solution which corresponds to the boundary chemical potential. Subsequently, the solution corresponding to the boundary magnetic field was also found [29].

In this paper, as a second problem, we shall formulate the graded reflection equation in terms of the fermionic $R$-matrix. It is shown explicitly that there are only two diagonal solutions for the graded reflection equation, which correspond to a) the boundary chemical potentials and b) the boundary magnetic fields. In this way, the integrability of the 1D Hubbard model with boundary fields (1.13) is proved. Moreover, making use of the covariance property of the reflection equation, we construct two non-diagonal solutions. It is shown that the partial particle-hole transformation for the fermionic $R$-matrix relates these solutions.

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§2. Fermionic R-Matrix and Graded Yang-Baxter Relation

Let us recall the fermionic formulation of the integrability of the 1D Hubbard model \[22, 23\]. The fermionic L-operator is given by

\[ \mathcal{L}_m(\theta) = \mathcal{L}(\theta)(\mathcal{L}_{m\uparrow}(\theta) \otimes \mathcal{L}_{m\downarrow}(\theta))\mathcal{L}(\theta), \tag{2.1} \]

where

\[ \mathcal{L}(\theta) = \cosh(\frac{\hbar}{2})I + \sinh(\frac{\hbar}{2})\sigma^z \otimes \sigma^z, \tag{2.2} \]

and

\[ \mathcal{L}_{m\uparrow}(\theta) = \left( \begin{array}{cc} -f_{m\uparrow}(\theta) & i\sigma^z f_{m\downarrow}(\theta) \\ i\sigma^z c_{m\downarrow}(\theta) & c_{m\uparrow}(\theta) \end{array} \right), \quad \mathcal{L}_{m\downarrow}(\theta) = \left( \begin{array}{cc} f_{m\downarrow}(\theta) & i\sigma^z c_{m\uparrow}(\theta) \\ -c_{m\downarrow}(\theta) & f_{m\uparrow}(\theta) \end{array} \right). \tag{2.3} \]

Here \( I \) is the \( 4 \times 4 \) identity matrix, \( \otimes \) means the usual direct product, and

\[ f_{ms}(\theta) = \sin \theta - \{ \sin \theta - i \cos \theta \} n_{ms}, \]
\[ g_{ms}(\theta) = \cos \theta - \{ \cos \theta + i \sin \theta \} n_{ms}. \tag{2.4} \]

The symbol \( \otimes \) denotes the Grassmann (graded) direct product

\[ [A \otimes B]_{\alpha\beta\gamma\delta} = (-1)^{[P(\alpha)+P(\beta)]P(\gamma)} A_{\alpha\beta} B_{\gamma\delta}, \]
\[ P(1) = 0, \quad P(2) = 1. \tag{2.5} \]

It is sometimes convenient to write the fermionic L-operator explicitly,

\[ \mathcal{L}_m(\theta) = \left( \begin{array}{cccc} -e^h f_{m\uparrow}(\theta) f_{m\downarrow}(\theta) & -f_{m\uparrow}(\theta)c_{m\downarrow} & i\sigma^z f_{m\downarrow}(\theta) & ie^h c_{m\uparrow}c_{m\downarrow} \\ -if_{m\uparrow}(\theta)c_{m\downarrow} & e^h f_{m\uparrow}(\theta)g_{m\downarrow}(\theta) & e^{-h} c_{m\uparrow}c_{m\downarrow} & ic_{m\uparrow}g_{m\downarrow}(\theta) \\ ic_{m\downarrow}f_{m\uparrow}(\theta) & e^{-h} c_{m\downarrow}c_{m\uparrow} & e^h g_{m\uparrow}(\theta)f_{m\downarrow}(\theta) & g_{m\uparrow}(\theta)c_{m\downarrow} \\ -ie^h c_{m\uparrow}c_{m\downarrow} & ic_{m\uparrow}g_{m\downarrow}(\theta) & ig_{m\uparrow}(\theta)c_{m\downarrow} & -e^h g_{m\uparrow}(\theta)g_{m\downarrow}(\theta) \end{array} \right). \tag{2.6} \]

The parameter \( h \) should be considered as a function of the spectral parameter \( \theta \) and the Coulomb coupling constant \( U \) through the relation

\[ \frac{\sinh 2h}{\sin 2\theta} = \frac{U}{4}. \tag{2.7} \]

The fermionic L-operator fulfills the graded Yang-Baxter relation \[22\]

\[ \hat{\mathcal{R}}_{12}(\theta_1, \theta_2)[\mathcal{L}_m(\theta_1) \otimes \mathcal{L}_m(\theta_2)] = [\mathcal{L}_m(\theta_2) \otimes \mathcal{L}_m(\theta_1)]\hat{\mathcal{R}}_{12}(\theta_1, \theta_2). \tag{2.8} \]

Here the parity of the Grassmann direct product \( \otimes \) is assigned as

\[ P(1) = P(4) = 0, \quad P(2) = P(3) = 1. \tag{2.9} \]

In the graded Yang-Baxter relation \[22, 23\], the constraints

\[ \frac{\sinh 2h_1}{\sin 2\theta_1} = \frac{\sinh 2h_2}{\sin 2\theta_2} = \frac{U}{4}, \tag{2.10} \]
are assumed. The matrix elements of the fermionic $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$ are given in ref. 22. For later use, we introduce an equivalent fermionic $R$-matrix

$$\mathcal{R}_{12}(\theta_1, \theta_2) \equiv \mathcal{P}_{12} \mathcal{R}_{12}(\theta_1, \theta_2), \quad (2.11)$$

where $\mathcal{P}_{12}$ is the graded permutation

$$\mathcal{P}_{\alpha\gamma;\beta\delta} = (-1)^{P(\alpha)P(\gamma)} \delta_{a\delta} \delta_{\gamma\beta}. \quad (2.12)$$

Using the fermionic $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$, the graded Yang-Baxter relation (2.8) can be expressed as

$$\mathcal{R}_{12}(\theta_1, \theta_2) \left( \mathcal{L}_m(\theta_1) \otimes I \right) \left( I \otimes \mathcal{L}_m(\theta_2) \right) = \left( I \otimes \mathcal{L}_m(\theta_2) \right) \left( \mathcal{L}_m(\theta_1) \otimes I \right) \mathcal{R}_{12}(\theta_1, \theta_2). \quad (2.13)$$

We parametrize the matrix elements of the fermionic $R$-matrix as follows

$$\mathcal{R}_{12}(\theta_1, \theta_2) = \begin{pmatrix}
  a^+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & -ib^+ & 0 & 0 & e & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & -ib^+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & -c^+ & 0 & 0 & if & 0 & 0 & -if & 0 & 0 & d^+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & e & 0 & 0 & ib^- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & -a^- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & if & 0 & 0 & c^- & 0 & 0 & -d^- & 0 & 0 & -if & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & ib^- & 0 & 0 & 0 & 0 & 0 & e & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & e & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & -if & 0 & 0 & 0 & 0 & c^- & 0 & 0 & -d^- & 0 & 0 & if & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & -a^- & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & d^+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & e & 0 & 0 & -ib^+ & 0 \\
  0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a^+ \\
\end{pmatrix}, \quad (2.14)$$

where

$$a^\pm = \cos^2(\theta_1 - \theta_2) \left\{ 1 \pm \tanh(h_1 - h_2) \frac{\cos(\theta_1 + \theta_2)}{\cos(\theta_1 - \theta_2)} \right\},$$

$$b^\pm = \sin(\theta_1 - \theta_2) \cos(\theta_1 - \theta_2) \left\{ 1 \pm \tanh(h_1 - h_2) \frac{\sin(\theta_1 + \theta_2)}{\sin(\theta_1 - \theta_2)} \right\},$$

$$c^\pm = \sin^2(\theta_1 - \theta_2) \left\{ 1 \pm \tanh(h_1 + h_2) \frac{\sin(\theta_1 + \theta_2)}{\sin(\theta_1 - \theta_2)} \right\},$$

$$d^\pm = 1 \pm \tanh(h_1 - h_2) \frac{\cos(\theta_1 - \theta_2)}{\cos(\theta_1 + \theta_2)}.$$
The second equalities for the Boltzmann weights \( b^\pm \) and \( d^\pm \) are due to the constraints (2.10), or equivalently the relation
\[
\frac{\tanh(h_1 - h_2)}{\tanh(h_1 + h_2)} = \frac{\tan(\theta_1 - \theta_2)}{\tan(\theta_1 + \theta_2)}.
\] (2.16)

We note some useful relations among the Boltzmann weights [22],
\[
d^\pm = a^\pm + c^\pm, \quad d^+d^- = e^2 + f^2,
\]
\[
e^2 = a^+a^- + b^+b^-, \quad f^2 = b^+b^- + c^+c^-.
\] (2.17)

The monodromy matrix is defined as the ordered product of the fermionic \( L \)-operators
\[
T(\theta) = \prod_{m=1}^{N} L_m(\theta) = L_N(\theta) \cdots L_1(\theta).
\] (2.18)

From the (local) graded Yang-Baxter relation (2.8), we have the global relation for the monodromy matrix
\[
\mathcal{R}_{12}(\theta_1, \theta_2)[T(\theta_1) \otimes_s T(\theta_2)] = [T(\theta_2) \otimes_s T(\theta_1)] \mathcal{R}_{12}(\theta_1, \theta_2),
\] (2.19)
or equivalently
\[
\mathcal{R}_{12}(\theta_1, \theta_2) \hat{T}^{-1}(\theta_1) \hat{T}^{-2}(\theta_2) = \hat{T}^{-2}(\theta_2) \hat{T}^{-1}(\theta_1) \mathcal{R}_{12}(\theta_1, \theta_2),
\] (2.20)

where
\[
\hat{T}^{-1}(\theta) \equiv T(\theta_1) \otimes I, \quad \hat{T}^{-2}(\theta) \equiv I \otimes T(\theta_2).
\] (2.21)

In other words, the monodromy matrix (2.18) is a representation of the associative algebra \( T \) defined by (2.19) or (2.20).

By taking the supertrace of (2.19) or (2.20), we find that the transfer matrix
\[
t(\theta) = \text{str}T(\theta) \equiv \text{tr} \{(\sigma^z \otimes \sigma^z) T(\theta)\}
\] (2.22)
constitutes a commuting family
\[
[t(\theta_1), t(\theta_2)] = 0.
\] (2.23)

Olmedilla et al. [22] showed that the Hamiltonian (1.1) under the periodic boundary condition (1.2) can be obtained by the series expansion of the transfer matrix \( t(\theta) \) around \( \theta = 0 \).

Now we list some properties enjoyed by the fermionic \( R \)-matrix \( \mathcal{R}_{12}(\theta_1, \theta_2) \).

(1) Regularity (Initial condition):
\[
\mathcal{R}_{12}(\theta_0, \theta_0) = \mathcal{P}_{12}.
\] (2.24)

(2) Graded Yang-Baxter equation:
\[
\mathcal{R}_{12}(\theta_1, \theta_2)\mathcal{R}_{13}(\theta_1, \theta_3)\mathcal{R}_{23}(\theta_2, \theta_3) = \mathcal{R}_{23}(\theta_2, \theta_3)\mathcal{R}_{13}(\theta_1, \theta_3)\mathcal{R}_{12}(\theta_1, \theta_2),
\] (2.25)

where we assume the constraints
\[
\frac{\sin 2h_1}{\sin 2\theta_1} = \frac{\sin 2h_2}{\sin 2\theta_2} = \frac{\sin 2h_3}{\sin 2\theta_3} = \frac{U}{4}.
\] (2.26)
(3) Unitarity:

\[ R_{12}(\theta_1, \theta_2)R_{21}(\theta_2, \theta_1) = \rho(\theta_1, \theta_2) \ I, \]  

where

\[ R_{21}(\theta_2, \theta_1) \equiv \mathcal{P}_{12}R_{12}(\theta_2, \theta_1)\mathcal{P}_{12}, \]  

and

\[ \rho(\theta_1, \theta_2) = \cos^2(\theta_1 - \theta_2) \{ \cos^2(\theta_1 - \theta_2) - \tanh^2(h_1 - h_2) \cos^2(\theta_1 + \theta_2) \}. \] (2.29)

(4) Crossing unitarity:

\[ R_{i2}^{st}(\theta_1, \theta_2)R_{i2}^{st}(\theta_2, -\theta_1) = R_{i2}^{st}(\theta_1, \theta_2)R_{i2}^{st}(\theta_2, -\theta_1) = \bar{\rho}(\theta_1, \theta_2) \ I, \]  

where

\[ \bar{\rho}(\theta_1, \theta_2) = \sin^2(\theta_1 + \theta_2) \{ \sin^2(\theta_1 + \theta_2) - \tanh^2(h_1 - h_2) \sin^2(\theta_1 - \theta_2) \}. \] (2.31)

Here the supertransposition acts on the 4 \times 4 matrix with the parity (2.33) as follows

\[
\begin{pmatrix}
D_{11} & C_{11} & C_{12} & D_{12} \\
B_{11} & A_{11} & A_{12} & B_{12} \\
B_{21} & A_{21} & A_{22} & B_{22} \\
D_{21} & C_{21} & C_{22} & D_{22}
\end{pmatrix}^\text{st} =
\begin{pmatrix}
D_{11} & -B_{11} & -B_{21} & D_{21} \\
C_{11} & A_{11} & A_{21} & C_{21} \\
C_{12} & A_{12} & A_{22} & C_{22} \\
D_{12} & -B_{12} & -B_{22} & D_{22}
\end{pmatrix}
\] (2.32)

In (2.30), st\textsubscript{j} means the supertransposition with respect to the j-th space.

We further note some properties of the R-matrix,

\[ R_{12}(\theta_1, \theta_2) = R_{12}(\theta_1 + \frac{\pi}{2}, \theta_2 + \frac{\pi}{2}) = \rho(\theta_1, \theta_2), \] (2.33)

\[ R_{12}(\theta_1, \theta_2)^{st_{1},st_{2}} = R_{12}(\theta_1, \theta_2)^{st_{1},st_{2}}. \] (2.34)

Here st\textsubscript{j} stands for the inverse of the supertransposition st\textsubscript{j},

\[ (X^{st})^{st} = (X^{\overline{st}})^{st} = X. \] (2.35)

We remark that $R_{12}(\theta_1, \theta_2)^{st_{1},st_{2}}$ can be obtained from the R-matrix $R_{12}(\theta_1, \theta_2)$ by exchanging the Boltzmann weights as if $\leftrightarrow -if$.

The graded tensor product is assumed in the above relations. The graded Yang-Baxter equation, for instance, is expressed as follows [31]

\[
R_{ab\theta'}(\theta_1, \theta_2)R_{a'c'\theta'}(\theta_1, \theta_3)R_{b'c'd}(\theta_2, \theta_3)(-)^{P(\theta')P(j)} = R_{b'c'\theta'}(\theta_2, \theta_3)R_{ac'd}(\theta_1, \theta_3)R_{a'\theta'j}(\theta_1, \theta_2)(-)^{P(\theta')P(a')} .
\] (2.36)

The authors gave a proof of the Yang-Baxter equation for Shastry’s R-matrix [24, 20]. We can show that the graded Yang-Baxter equation for the fermionic R-matrix is equivalent to the Yang-Baxter equation for Shastry’s R-matrix.
§3. Symmetry of the Fermionic $R$-Matrix and Twisted Periodic Boundary Condition

In this section we shall discuss two important symmetries of the fermionic $R$-matrix. The symmetry of the fermionic $R$-matrix is defined by the constant matrix $M = (M_{ij})$ that satisfies

$$\left[\mathcal{R}_{12}(\theta_1, \theta_2), M \otimes M\right] = 0,$$

or equivalently,

$$\mathcal{R}_{12}(\theta_1, \theta_2)(M \otimes I)(I \otimes M) = (I \otimes M)(M \otimes I)\mathcal{R}_{12}(\theta_1, \theta_2).$$

(3.1)

(3.2)

Here we assume that the matrix elements $M_{ij}$ are commuting numbers. Solving the defining relation (3.1) or (3.2), we have found that the symmetry matrix $M$ for the fermionic $R$-matrix takes the following form

$$M = \begin{pmatrix} M_{11} & 0 & 0 & M_{14} \\ 0 & M_{22} & M_{23} & 0 \\ 0 & M_{32} & M_{33} & 0 \\ M_{41} & 0 & 0 & M_{44} \end{pmatrix},$$

(3.3)

with the condition

$$M_{11}M_{44} - M_{14}M_{41} = M_{22}M_{33} - M_{23}M_{32}.$$  

(3.4)

We denote the submatrices of $M$ as

$$M_{\text{charge}} = \begin{pmatrix} M_{11} & M_{14} \\ M_{41} & M_{44} \end{pmatrix}, M_{\text{spin}} = \begin{pmatrix} M_{22} & M_{23} \\ M_{32} & M_{33} \end{pmatrix}.$$  

(3.5)

Then the condition (3.4) can be written

$$\det M_{\text{charge}} = \det M_{\text{spin}} \equiv \Delta(M).$$  

(3.6)

Since an overall constant is not relevant for the integrability, we put

$$\Delta(M) = 1.$$  

(3.7)

In other words, the submatrices $M_{\text{charge}}, M_{\text{spin}}$ belong to $SL(2, \mathbb{C})$. The symmetry matrix $M$ reflects the $SO(4)$ symmetry of the Hamiltonian. It is to be remarked that the symmetry matrix $\tilde{M}$ of Shastry’s $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$, which is defined by

$$\left[\mathcal{R}_{12}(\theta_1, \theta_2), \tilde{M} \otimes \tilde{M}\right] = 0,$$

is not of the form (3.3) and (3.4) [31]. Shastry’s $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$ is related to the fermionic $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$ through the formula [22]

$$\mathcal{R}_{12}(\theta_1, \theta_2) = W_{12}^{-1}\mathcal{R}_{12}(\theta_1, \theta_2)W_{12},$$

(3.8)
where $W_{12}$ is a diagonal $16 \times 16$ matrix

$$W_{12} = \text{diag}(1, 1, -i, -i, -i, -i, 1, 1, -1, -1, i, i, i, -1, -1).$$  (3.10)

Since (3.9) is not a gauge transformation, the symmetry of Shastry’s $R$-matrix may be different from that of the fermionic $R$-matrix. The fermionic $R$-matrix is more suitable when we investigate the symmetry of the fermionic Hamiltonian in the framework of the QISM.

Using the symmetry matrix, one may twist the periodic boundary condition. The symmetry matrix $M$ can be inserted into the transfer matrix without breaking the integrability [27]

$$t(\theta; M) = \text{str} \{MT(\theta)\}. \quad (3.11)$$

The generalized transfer matrix $t(\theta; M)$ still constitutes a commuting family

$$[t(\theta_1; M), t(\theta_2; M)] = 0. \quad (3.12)$$

The series expansion of $t(\theta; M)$ around $\theta = 0$ gives rise to a Hamiltonian $\hat{H}(M)$

$$t(\theta; M) = \text{str} \{MT(0)\} (1 + \theta \hat{H}(M) + \cdots) \quad (3.13)$$

where

$$\hat{H}(M) = -\sum_{m=1}^{N-1} \sum_{s=\downarrow} (c_{ms}^\dagger c_{m+1s} + c_{m+1s}^\dagger c_{ms}) + U \sum_{m=1}^{N} (n_{m\uparrow} - \frac{1}{2})(n_{m\downarrow} - \frac{1}{2})
- (M_{11} M_{22}^\dagger c_{1\uparrow} + iM_{11} M_{32}^\dagger c_{1\downarrow} - M_{41} M_{32}^\dagger c_{1\uparrow} - iM_{41} M_{22}^\dagger c_{1\downarrow})c_{N\uparrow}
- c_{N\uparrow}^\dagger (M_{33} M_{44}^\dagger c_{1\downarrow} + iM_{44} M_{23}^\dagger c_{1\uparrow} - M_{14} M_{23}^\dagger c_{1\downarrow} - iM_{14} M_{33}^\dagger c_{1\uparrow})
- (M_{11} M_{33}^\dagger c_{1\downarrow} - iM_{11} M_{23}^\dagger c_{1\uparrow} - M_{41} M_{23}^\dagger c_{1\downarrow} + iM_{41} M_{33}^\dagger c_{1\uparrow})c_{N\downarrow}
- c_{N\downarrow}^\dagger (M_{22} M_{44}^\dagger c_{1\uparrow} - iM_{44} M_{32}^\dagger c_{1\downarrow} - M_{14} M_{32}^\dagger c_{1\downarrow} + iM_{14} M_{22}^\dagger c_{1\uparrow}). \quad (3.14)$$

It is easy to see that the choice $M = I$ corresponds to the periodic boundary condition [17, 22].

Further, we assume the submatrices $M_{\text{charge}}$ and $M_{\text{spin}}$ belong to $SU(2)$. Namely,

$$M_{44} = M_{11}^*, \quad M_{41} = -M_{14}^*, \quad |M_{11}|^2 + |M_{14}|^2 = 1, \quad (3.15)$$
$$M_{33} = M_{22}^*, \quad M_{32} = -M_{23}^*, \quad |M_{22}|^2 + |M_{23}|^2 = 1. \quad (3.16)$$

Here the symbol * means the complex conjugation. In this case, we find that the periodic boundary condition is twisted as follows

$$c_{N+1\uparrow}^\dagger = M_{11} M_{22}^\dagger c_{1\downarrow} - iM_{11} M_{32}^\dagger c_{1\downarrow} - M_{14}^* M_{23}^\dagger c_{1\uparrow} + iM_{14} M_{22}^\dagger c_{1\downarrow},$$
$$c_{N+1\uparrow} = M_{11}^* M_{22} c_{1\uparrow} + iM_{11} M_{23} c_{1\downarrow} - M_{14}^* M_{23}^\dagger c_{1\uparrow} - iM_{14} M_{22} c_{1\downarrow},$$
$$c_{N+1\downarrow}^\dagger = M_{11} M_{22}^\dagger c_{1\downarrow} - iM_{11} M_{23}^\dagger c_{1\downarrow} - M_{14}^* M_{23}^\dagger c_{1\uparrow} + iM_{14} M_{22}^\dagger c_{1\downarrow},$$
$$c_{N+1\downarrow} = M_{22} M_{11}^* c_{1\uparrow} + iM_{11} M_{23}^\dagger c_{1\uparrow} - M_{14}^* M_{23} c_{1\downarrow} + iM_{14} M_{22} c_{1\downarrow}. \quad (3.17)$$
The relations (3.17) can be expressed in a matrix form
\[
\begin{pmatrix}
  c_{N+1\downarrow}^\dagger & i c_{N+1\uparrow} \\
  i c_{N+1\downarrow} & c_{N+1\downarrow}
\end{pmatrix}
= M^{-1}_{\text{spin}}
\begin{pmatrix}
  c_{1\downarrow}^\dagger & i c_{1\uparrow} \\
  i c_{1\downarrow} & c_{1\uparrow}
\end{pmatrix}
M_{\text{charge}}.
\]  
(3.18)

This shows that the periodic boundary condition can be rotated by the group \(SU(2) \times SU(2)\). A quite similar \(SO(4)\) rotation was observed by Affleck [7].

Since the choices \(M_{\text{spin}} = -1, M_{\text{charge}} = 1\) and \(M_{\text{spin}} = 1, M_{\text{charge}} = -1\) induce the same transformation (3.18), the exact group symmetry is \(SO(4) = [SU(2) \times SU(2)]/\mathbb{Z}_2\).

Now let us consider the diagonal \(M\) parametrized as follows,
\[
M = e^{i \phi \sigma_z} \otimes e^{i \psi \sigma_z}
= \begin{pmatrix}
  e^{i \phi} & 0 & 0 & 0 \\
  0 & e^{i \phi} & 0 & 0 \\
  0 & 0 & e^{-i \phi} & 0 \\
  0 & 0 & 0 & e^{-i \phi}
\end{pmatrix}.
\]  
(3.19)

From (3.17), the corresponding twisted periodic boundary condition is
\[
\begin{align*}
  c_{N+1\uparrow}^\dagger &= e^{i \phi} c_{1\uparrow}^\dagger, & c_{N+1\downarrow} &= e^{-i \phi} c_{1\uparrow}, \\
  c_{N+1\downarrow}^\dagger &= e^{i \psi} c_{1\downarrow}^\dagger, & c_{N+1\downarrow} &= e^{-i \psi} c_{1\downarrow},
\end{align*}
\]  
(3.20)

which is identical to (1.8). Especially, if we take \(\phi = \pi\) and \(\psi = -\pi\), (3.19) becomes
\[
M = \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & -1 & 0 & 0 \\
  0 & 0 & -1 & 0 \\
  0 & 0 & 0 & 1
\end{pmatrix} = \sigma^z \otimes \sigma^z.
\]  
(3.21)

In this case, the supertrace in the transfer matrix (3.11) becomes the usual trace
\[
\text{str} \{(\sigma^z \otimes \sigma^z) T(\theta)\} = \text{tr} T(\theta).
\]  
(3.22)

Thus, as remarked in ref. 23, we can take the trace of the monodromy matrix instead of the supertrace. However, the boundary condition in this case should be anti-periodic
\[
\begin{align*}
  c_{N+1\uparrow}^\dagger &= -c_{1\uparrow}^\dagger, & c_{N+1\downarrow} &= -c_{1\downarrow}, \\
  c_{N+1\downarrow}^\dagger &= -c_{1\downarrow}^\dagger, & c_{N+1\downarrow} &= -c_{1\downarrow}.
\end{align*}
\]  
(3.23)

Next we consider a discrete symmetry related to the partial particle-hole transformation (1.6). We solve the following equation
\[
\mathcal{R}_{12}(\theta_1, \theta_2; U)(N \otimes I)(I \otimes N) = (I \otimes N)(N \otimes I)\mathcal{R}_{12}(\theta_1, \theta_2; -U).
\]  
(3.24)

with a constant matrix \(N = (N_{ij})\). Here we explicitly write the \(U\)-dependence of the fermionic \(R\)-matrix. Note that the coupling constant of the fermionic \(R\)-matrix in the RHS is \(-U\), or
equivalently \( h_1 \rightarrow -h_1, h_2 \rightarrow -h_2 \). By solving the defining relation (3.24), we find that the constant matrix \( N \) has a form,

\[
N = \begin{pmatrix}
0 & N_{12} & N_{13} & 0 \\
N_{21} & 0 & 0 & N_{24} \\
N_{31} & 0 & 0 & N_{34} \\
0 & N_{42} & N_{43} & 0
\end{pmatrix},
\]

(3.25)

with a condition

\[
\Delta(N) = N_{12}N_{43} - N_{13}N_{42} = N_{21}N_{34} - N_{31}N_{24}.
\]

(3.26)

We set

\[
\Delta(N) = 1,
\]

(3.27)

as before. The matrix \( N \) can be written as

\[
N = (1 \otimes \sigma^x) \begin{pmatrix}
N_{21} & 0 & 0 & N_{24} \\
0 & N_{12} & N_{13} & 0 \\
0 & N_{42} & N_{43} & 0 \\
N_{31} & 0 & 0 & N_{34}
\end{pmatrix}.
\]

(3.28)

Here and hereafter, \( 1 \) means the \( 2 \times 2 \) identity matrix. Thus \( N \) is a composition of the symmetry matrix (3.3) and

\[
Q = Q^{-1} = 1 \otimes \sigma^x = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}.
\]

(3.29)

In terms of this matrix, the fermionic \( R \)-matrix with the coupling constant \( U \) is transformed into the fermionic \( R \)-matrix with the coupling constant \(-U\) as follows

\[
\frac{1}{2} Q^{-1} Q^{-1} R_{12}(\theta_1, \theta_2; U) \frac{1}{2} Q Q = R_{12}(\theta_1, \theta_2; -U).
\]

(3.30)

The matrix \( Q \) is related to the partial particle-hole transformation (1.6) of the Hamiltonian. There are other choices for the matrix \( Q \). For example,

\[
Q = \sigma^z \otimes \sigma^y = \begin{pmatrix}
0 & -i & 0 & 0 \\
i & 0 & 0 & 0 \\
0 & 0 & 0 & i \\
0 & 0 & -i & 0
\end{pmatrix}
\]

(3.31)

also satisfies (3.30), which may be more appropriate as the partial particle-hole transformation (1.6) [32]. However, for simplicity, we choose the matrix (3.29) as the partial particle-hole transformation of the fermionic \( R \)-matrix.
§4. Graded Reflection Equations for the Fermionic $R$-Matrix

In this section we investigate the integrability of the 1D Hubbard model with open boundary condition in terms of the fermionic $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$. We introduce an associative algebra $\mathcal{T}_-$ defined by the fermionic $R$-matrix $\mathcal{R}_{12}(\theta_1, \theta_2)$, 

$$\mathcal{R}_{12}(\theta_1, \theta_2) \frac{1}{\mathcal{T}_-(\theta_1)} \mathcal{R}_{21}(\theta_2, -\theta_1) \frac{2}{\mathcal{T}_-(\theta_2)} = \frac{2}{\mathcal{T}_-(\theta_2)} \mathcal{R}_{12}(\theta_1, -\theta_2) \frac{1}{\mathcal{T}_-(\theta_1)} \mathcal{R}_{21}(-\theta_2, -\theta_1), \quad (4.1)$$

where

$$\frac{1}{\mathcal{T}_-(\theta_1)} \equiv \mathcal{T}_-(-\theta_1) \otimes I, \quad \frac{2}{\mathcal{T}_-(\theta_2)} \equiv I \otimes \mathcal{T}_-(\theta_2). \quad (4.2)$$

The relation (4.1) is called the graded reflection equation (graded RE).

The following theorem is fundamental for the application of the associative algebra $\mathcal{T}_-$. 

Theorem $[27, 34]$

Let $\mathcal{T}_-(\theta)$ be some representation of the associative algebra $\mathcal{T}_- (1.1)$ and $T(\theta)$ of the associative algebra $T (2.20)$. Then $\mathcal{T}_-(\theta)$ defined by

$$\mathcal{T}_-(\theta) = T(\theta) \mathcal{T}_-(\theta) T^{-1}(-\theta), \quad (4.3)$$

is also a representation of $\mathcal{T}_-$ provided that the matrix elements of $\mathcal{T}_-(\theta)$ and $T(\theta)$ commute. This property is sometimes called the covariance property of the (graded) reflection equation $[34]$. For the application to the 1D Hubbard model, we choose $T(\theta)$ and $\mathcal{T}_-(\theta)$ as

$$T(\theta) = L_N(\theta) L_{N-1}(\theta) \cdots L_1(\theta),$$

$$\mathcal{T}_-(\theta) = K_-(\theta). \quad (4.4)$$

Here $K_-(\theta)$ is a constant supermatrix satisfying the graded RE (1.1),

$$\mathcal{R}_{12}(\theta_1, \theta_2) \frac{1}{K_-(\theta_1)} \mathcal{R}_{21}(\theta_2, -\theta_1) \frac{2}{K_-(\theta_2)} = \frac{2}{K_-(\theta_2)} \mathcal{R}_{12}(\theta_1, -\theta_2) \frac{1}{K_-(\theta_1)} \mathcal{R}_{21}(-\theta_2, -\theta_1). \quad (4.5)$$

The $K$-matrix $K_-(\theta)$ specifies the integrable boundary condition. In this paper we assume that the matrix elements of $K_-(\theta)$ are commuting numbers and only the even elements with respect to the parity (2.9) are non zero $[33]$, 

$$K_-(\theta) = \begin{pmatrix} K_{11}(\theta) & 0 & 0 & K_{14}(\theta) \\ 0 & K_{22}(\theta) & K_{23}(\theta) & 0 \\ 0 & K_{32}(\theta) & K_{33}(\theta) & 0 \\ K_{41}(\theta) & 0 & 0 & K_{44}(\theta) \end{pmatrix}. \quad (4.6)$$

To construct a transfer matrix, we introduce another $K$-matrix $K_+(\theta)$ satisfying the conjugated graded RE

$$\mathcal{R}_{21}^{st_1, st_2}(\theta_2, \theta_1) \frac{1}{K_+(\theta_1)} \mathcal{R}_{12}^{st_1, st_2}(-\theta_1, \theta_2) \frac{2}{K_+(\theta_2)} = \frac{2}{K_+(\theta_2)} \mathcal{R}_{21}^{st_1, st_2}(-\theta_2, \theta_1) \frac{1}{K_+(\theta_1)} \mathcal{R}_{12}^{st_1, st_2}(-\theta_1, -\theta_2). \quad (4.7)$$
We assume that the \( K \)-matrix \( K_+(\theta) \) is also of the form (4.3). Then the supertransposition to the \( K \)-matrix \( K_+(\theta) \) reduce to the usual transposition.

Now we define the transfer matrix by

\[
\tau(\theta) = \text{str} \{ K_+(\theta) T_-(\theta) \} = \text{str} \{ K_+(\theta) T(\theta) K_-(\theta) T^{-1}(\theta) \}. \tag{4.8}
\]

Using the unitarity (2.27), the crossing unitarity (2.30) and the graded REs (4.1), (4.7), we can show that the transfer matrix \( \tau(\theta) \) constitutes a commutative family [27], i.e.,

\[
[\tau(\theta_1), \tau(\theta_2)] = 0, \tag{4.9}
\]

which shows the existence of the mutually commuting conserved currents including the Hamiltonian.

We note

\[
T^{-1}(\theta) = L_1^{-1}(\theta) \cdots L_N^{-1}(\theta), \tag{4.10}
\]

where

\[
L_{m}^{-1}(\theta) = \frac{1}{\cos^4 \theta} \left( \begin{array}{cccc}
-e^h f_{m\uparrow}^*(\theta) f_{m\downarrow}^*(\theta) & if_{m\uparrow}^*(\theta) c_{m\downarrow} & c_{m\uparrow} f_{m\downarrow}^*(\theta) & -ie^h c_{m\uparrow} c_{m\downarrow} \\
-f_{m\uparrow}^*(\theta) c_{m\downarrow} & e^{-h} f_{m\uparrow}^*(\theta) g_{m\downarrow}(\theta) & -e^{-h} c_{m\uparrow} c_{m\downarrow} & c_{m\uparrow} g_{m\downarrow}(\theta) \\
-ic_{m\uparrow}^* f_{m\downarrow}(\theta) & -e^{-h} c_{m\uparrow} c_{m\downarrow} & e^{-h} g_{m\uparrow}(\theta) f_{m\downarrow}^*(\theta) & -ig_{m\uparrow}(\theta) c_{m\downarrow} \\
ie^h c_{m\uparrow}^* c_{m\downarrow} & -ic_{m\uparrow}^* g_{m\downarrow}(\theta) & g_{m\uparrow}(\theta) c_{m\downarrow} & -e^h g_{m\uparrow}(\theta) g_{m\downarrow}(\theta)
\end{array} \right)
\]

\[
= \frac{1}{\cos^4 \theta} \mathcal{L}(\theta) \left( \bar{L}_{m\uparrow}(\theta) \otimes \bar{L}_{m\downarrow}(\theta) \right) \mathcal{L}(\theta). \tag{4.11}
\]

Here we define

\[
\bar{L}_{m\uparrow}(\theta) = \left( \begin{array}{cc}
-f_{m\uparrow}^*(\theta) & c_{m\uparrow} \\
-ic_{m\uparrow}^* & g_{m\uparrow}(\theta)
\end{array} \right), \quad \bar{L}_{m\downarrow}(\theta) = \left( \begin{array}{cc}
f_{m\downarrow}(\theta) & -ic_{m\downarrow} \\
c_{m\downarrow} & -g_{m\downarrow}(\theta)
\end{array} \right). \tag{4.12}
\]

§5. Integrability of the 1D Hubbard Model with Boundary Fields

In this section we solve the graded REs (4.3) and (4.7) for \( K_-(\theta) \) and \( K_+(\theta) \). First, we note a relation between the \( R \)-matrix

\[
R_{12}(\theta_1, \theta_2) = R_{21}^*(\theta_2, -\theta_1). \tag{5.1}
\]

Then the graded RE (4.3) for \( K_-(\theta) \) is cast into a form

\[
\mathcal{R}_{12}(\theta_1, \theta_2) K_-(\theta_1) \mathcal{R}_{12}^*(\theta_1, -\theta_2) K_-(\theta_2) = \frac{1}{2} K_-(\theta_2) \mathcal{R}_{12}(\theta_1, -\theta_2) K_-(\theta_1) \mathcal{R}_{12}^*(\theta_1, \theta_2), \tag{5.2}
\]
with the graded tensor products,
\[
\tilde{K}_-(\theta_1) \equiv K_-(\theta_1) \otimes I,
\quad \tilde{K}_-(\theta_2) \equiv I \otimes K_-(\theta_2).
\] (5.3)

Assuming \( K_-(\theta) \) in a diagonal form
\[
K_-(\theta) = \begin{pmatrix}
  x_1(\theta) & 0 & 0 & 0 \\
  0 & x_2(\theta) & 0 & 0 \\
  0 & 0 & x_3(\theta) & 0 \\
  0 & 0 & 0 & x_4(\theta)
\end{pmatrix},
\] (5.4)

and substituting it into the graded RE (5.2), we have 10 non-trivial functional equations for \( x_i(\theta), (i = 1, \cdots 4) \). By solving these functional equations (see Appendix), we obtain the following two sets of solutions for the diagonal \( K_-(\theta) \).

a) \( K_-(\theta) = K_-(a)(\theta; p_-) \):
\[
\begin{align*}
  x_1(\theta) &= \left( 1 - p_-e^{-2h} \tan \theta \right) \left( 1 - p_-e^{2h} \tan \theta \right), \\
  x_2(\theta) &= x_3(\theta) = e^{-2h} \left( 1 + p_-e^{2h} \tan \theta \right) \left( 1 - p_-e^{2h} \tan \theta \right), \\
  x_4(\theta) &= \left( 1 + p_-e^{2h} \tan \theta \right) \left( 1 + p_-e^{-2h} \tan \theta \right).
\end{align*}
\] (5.5)

b) \( K_-(\theta) = K_-(b)(\theta; p_-) \):
\[
\begin{align*}
  x_1(\theta) &= x_4(\theta) = e^{2h} \left( 1 + p_-e^{-2h} \tan \theta \right) \left( 1 - p_-e^{-2h} \tan \theta \right), \\
  x_2(\theta) &= \left( 1 - p_-e^{-2h} \tan \theta \right) \left( 1 - p_-e^{2h} \tan \theta \right), \\
  x_3(\theta) &= \left( 1 + p_-e^{-2h} \tan \theta \right) \left( 1 + p_-e^{2h} \tan \theta \right).
\end{align*}
\] (5.6)

Here \( p_- \) is a constant parameter corresponding to the boundary field. Recall that the parameter \( h \) is regarded as a function of the spectral parameter \( \theta \) through the constraint
\[
\frac{\sinh 2h}{\sin 2\theta} = \frac{U}{4}.
\] (5.7)

When we put \( p_- = 0 \), the solutions \( K_-(a)(\theta; p_-) \) and \( K_-(b)(\theta; p_-) \) are proportional to \( L^2(\theta) \),
\[
\begin{align*}
  K_-(a)(\theta; p_- = 0) &= e^{-h} \mathcal{L}^2(\theta), \\
  K_-(b)(\theta; p_- = 0) &= e^h \mathcal{L}^2(\theta),
\end{align*}
\] (5.8) (5.9)

which supply the missing interaction term at the boundary site \( m = 1 \). To see the contributions of the boundary fields clearly, we redefine
\[
\begin{align*}
  \tilde{K}-(a)(\theta; p_-) &= e^h \mathcal{L}^{-1}(\theta)K_-(a)(\theta; p_-)\mathcal{L}^{-1}(\theta), \\
  \tilde{K}-(b)(\theta; p_-) &= e^{-h} \mathcal{L}^{-1}(\theta)K_-(b)(\theta; p_-)\mathcal{L}^{-1}(\theta).
\end{align*}
\] (5.10) (5.11)

Expanding \( \tilde{K}_-(a)(\theta; p_-) \) around \( \theta = 0 \), we have
\[
\tilde{K}_-(a)(\theta; p_-) = 1 \otimes 1 - p_- (\sigma^z \otimes 1 + 1 \otimes \sigma^z) \theta + \cdots.
\] (5.12)
Now the linear term with respect to the spectral parameter produces the boundary chemical potential at the site $m = 1$

$$ - p_-(n_{1\uparrow} + n_{1\downarrow} - 1). \quad (5.13) $$

Similarly, we have

$$ \tilde{K}_-(\theta; p_-) = 1 \otimes 1 - p_-(\sigma^z \otimes 1 - 1 \otimes \sigma^z) \theta + \cdots. \quad (5.14) $$

The linear term in (5.14) gives the boundary magnetic field at the site $m = 1$

$$ - p_-(n_{1\uparrow} - n_{1\downarrow}). \quad (5.15) $$

Thus we have shown that $K_-(a; \theta; p_-)$ corresponds to the boundary chemical potential, while $K_-(b; \theta; p_-)$ corresponds to the boundary magnetic field.

A comment is in order on the derivations of (5.13) and (5.15). Rigorously speaking, (5.12) and (5.14) respectively give twice of (5.13) and (5.15). However, the bulk Hamiltonian appears twice in the expansion of the transfer matrix. Therefore the Hamiltonian contains the boundary fields as given in (5.13) and (5.15).

We also remark that the diagonal solutions (5.5) and (5.6) coincide with those found for the coupled spin model (1.15) \cite{28, 29}. Actually, if we formulate the reflection equation in terms of Shastry’s $R$-matrix \cite{28}, we obtain the same functional equations as (A.5)–(A.14) (see Appendix) for the diagonal $K_-(\theta)$.

Solving the graded RE (4.7) for the diagonal $K_+(\theta)$ in a similar way, we obtain two solutions for the $K$-matrix $K_+(\theta)$ as follow.

a) $K_+(\theta) = K_+(a; \theta; p_+)$:

\begin{align*}
x_1(\theta) &= (p_+ + e^{2h} \tan \theta) \left( p_+ + e^{-2h} \tan \theta \right), \\
x_2(\theta) &= x_3(\theta) = e^{2h} \left( p_+ + e^{-2h} \tan \theta \right) \left( p_+ - e^{-2h} \tan \theta \right) \\
x_4(\theta) &= (p_+ - e^{2h} \tan \theta) \left( p_+ - e^{-2h} \tan \theta \right). \quad (5.16)
\end{align*}

b) $K_+(\theta) = K_+(b; \theta; p_+)$:

\begin{align*}
x_1(\theta) &= x_4(\theta) = e^{-2h} \left( p_+ + e^{2h} \tan \theta \right) \left( p_+ - e^{2h} \tan \theta \right), \\
x_2(\theta) &= (p_+ + e^{2h} \tan \theta) \left( p_+ + e^{-2h} \tan \theta \right), \\
x_3(\theta) &= (p_+ - e^{2h} \tan \theta) \left( p_+ - e^{-2h} \tan \theta \right). \quad (5.17)
\end{align*}

In (5.16) and (5.17), the parameter $p_+$ represents the strength of the boundary field at the site $m = N$. The solution $K_+(a; \theta; p_+)$ corresponds to the boundary chemical potential and $K_+(b; \theta; p_+)$ corresponds to the boundary magnetic field.

As in the case of (5.10) and (5.11), we may redefine

\begin{align*}
\tilde{K}_+(a; \theta; p_+) &= e^{-h} \mathcal{L}(\theta) K_+(a; \theta; p_+) \mathcal{L}(\theta), \\
\tilde{K}_+(b; \theta; p_+) &= e^{h} \mathcal{L}(\theta) K_+(b; \theta; p_+) \mathcal{L}(\theta). \quad (5.18)
\end{align*}
Then around $\theta = 0$, we have

$$
\tilde{K}_+^{(a)}(\theta; p_+) = p_+^2 \left( 1 \otimes 1 \right) + p_+ \left( \sigma^z \otimes 1 + 1 \otimes \sigma^z \right) \theta + (\sigma^z \otimes \sigma^z) \theta^2 + \cdots \quad (5.20)
$$

$$
\tilde{K}_+^{(b)}(\theta; p_+) = p_+^2 \left( 1 \otimes 1 \right) + p_+ \left( \sigma^z \otimes 1 - 1 \otimes \sigma^z \right) \theta - (\sigma^z \otimes \sigma^z) \theta^2 + \cdots \quad (5.21)
$$

From (5.20) and (5.21), we find the following properties

$$
\text{str} \tilde{K}_+^{(a)}(\theta = 0; p_+) = \text{str} \tilde{K}_+^{(b)}(\theta = 0; p_+) = 0, \quad (5.22)
$$

$$
\text{str} \left( \frac{d}{d\theta} \tilde{K}_+^{(a)}(\theta; p_+) \bigg|_{\theta = 0} \right) = \text{str} \left( \frac{d}{d\theta} \tilde{K}_+^{(b)}(\theta; p_+) \bigg|_{\theta = 0} \right) = 0. \quad (5.23)
$$

Using the solutions (5.3), (5.6), (5.16) and (5.17), we can construct the four integrable transfer matrices $\tau(\theta) = \text{str} \{ K_+^{(a)}(\theta) T(\theta) K_-^{(a)}(\theta) T^{-1}(\theta) \}$.

Case A. \( K_-^{(a)}(\theta) = K_+^{(a)}(\theta; p_1), \quad K_+^{(a)}(\theta) = K_+^{(a)}(\theta; p_N). \)

Case B. \( K_-^{(b)}(\theta) = K_+^{(b)}(\theta; p_1), \quad K_+^{(b)}(\theta) = K_+^{(b)}(\theta; p_N). \)

Case C. \( K_-^{(a)}(\theta) = K_+^{(a)}(\theta; p_1), \quad K_+^{(a)}(\theta) = K_+^{(a)}(\theta; p_N). \)

Case D. \( K_-^{(a)}(\theta) = K_+^{(a)}(\theta; p_1), \quad K_+^{(a)}(\theta) = K_+^{(b)}(\theta; p_N). \) \quad (5.24)

These results are consistent with the coordinate Bethe ansatz for the cases (1.10). The Hamiltonian (1.9) is obtained by expanding the transfer matrix with respect to the spectral parameter $\theta$

$$
\tau(\theta) = C_1 \theta + C_2 \theta^2 + C_3 \left( \tilde{H}_{\text{open}} + \text{const.} \right) \theta^3 + \cdots. \quad (5.25)
$$

Here $C_i \ (i = 1, 2, 3, \cdots)$ are some scalar functions. We omit the detailed derivation of (5.25) in this paper, which can be carried out using the method in ref. 22. Due to the properties (5.22) and (5.23), the Hamiltonian $\tilde{H}_{\text{open}}$ appears at the third order of the expansion.

The commutativity of the transfer matrix

$$
[\tau(\theta_1), \tau(\theta_2)] = 0 \quad (5.26)
$$

ensures the existence of an infinite number of the conserved currents in involution. The exact integrability of the 1D Hubbard model with the boundary fields (1.3) is established in this way.

The $K$-matrices (5.16) and (5.17) are slightly different from those for Shastry’s $R$-matrix \[28 \ 29\], which we denote $\tilde{K}_+(\theta)$. The former can be obtained from the latter by multiplying the diagonal matrix $\sigma^z \otimes \sigma^z$,

$$
K_+^{(a)}(\theta) = (\sigma^z \otimes \sigma^z) \tilde{K}_+(\theta). \quad (5.27)
$$

Due to the definition of the supertrace (2.22), both formulations provide the same transfer matrix

$$
\text{str} \left\{ K_+^{(a)}(\theta) T(\theta) K_-^{(a)}(\theta) T^{-1}(\theta) \right\} = \text{tr} \left\{ K_+^{(a)}(\theta) T(\theta) K_-^{(a)}(\theta) T^{-1}(-\theta) \right\}. \quad (5.28)
$$
Non-Diagonal Solutions of the Graded Reflection Equation

We can construct non-diagonal solutions of the graded RE (4.5) by use of the covariance property (4.3) and the symmetry matrix \( M \). For example, we have a solution

\[
K_-(\theta; p_-, M_{\text{charge}}) = MK_-(\theta; p_-)M^{-1}
\]

where

\[
\begin{align*}
K_{11}(\theta) &= 1 - 2p_-(M_{11}M_{44} + M_{14}M_{41}) \cosh 2h \tan \theta + p_-^2 \tan^2 \theta, \\
K_{22}(\theta) &= K_{33}(\theta) = e^{-2h} \left( 1 - p_-^2 e^{4h} \tan^2 \theta \right), \\
K_{44}(\theta) &= 1 + 2p_-(M_{11}M_{44} + M_{14}M_{41}) \cosh 2h \tan \theta + p_-^2 \tan^2 \theta, \\
K_{14}(\theta) &= 4p_- M_{11}M_{14} \cosh 2h \tan \theta, \\
K_{41}(\theta) &= -4p_- M_{41}M_{44} \cosh 2h \tan \theta.
\end{align*}
\]  

(6.1)

Note that \( K_-(\theta; p_-, M_{\text{charge}}) \) does not depend on the submatrix \( M_{\text{spin}} \).

Since the relation

\[
M_{11}M_{44} + M_{14}M_{41} = \left\{ (M_{11}M_{44} - M_{14}M_{41})^2 + 4M_{11}M_{14}M_{41}M_{44} \right\}^{\frac{1}{2}}
\]

(6.2)

holds, the solution (6.2) depends on three arbitrary parameters,

\[
p_-, \quad \alpha = M_{11}M_{14}, \quad \beta = -M_{41}M_{44}.
\]  

(6.3)

The corresponding boundary term is

\[
-p_-( (M_{11}M_{44} + M_{14}M_{41}) (n_{l\uparrow} + n_{l\downarrow} - 1) - 2iM_{11}M_{14} c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger - 2iM_{41}M_{44} c_{1\downarrow}^\dagger c_{1\uparrow} )
\]

(6.4)

\[
= -p_- \{ (1 - 4\alpha \beta) \left( n_{l\uparrow} + n_{l\downarrow} - 1 \right) - 2i\alpha c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger + 2i\beta c_{1\downarrow}^\dagger c_{1\uparrow} \}.
\]  

(6.5)

Note the existence of the term \( c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger (c_{1\downarrow} c_{1\uparrow}) \) which creates (annihilates) a double occupied state at the boundary site. If we assume \( M_{\text{charge}} \in SU(2) \) (cf. (3.15)), we have

\[
\beta = \alpha^*,
\]  

(6.6)

and the boundary term (6.3) becomes hermitian (\( p_- \) is assumed to be real).

Similarly, we have

\[
K_-(\theta; p_-, M_{\text{spin}}) = MK_-(\theta; p_-)M^{-1}
\]

(6.7)
where

\[
K_{11}(\theta) = K_{44}(\theta) = e^{2h} \left( 1 - p_-^2 e^{-4h \tan^2 \theta} \right),
\]
\[
K_{22}(\theta) = 1 - 2p_- (M_{22} M_{33} + M_{23} M_{32}) \cosh 2h \tan \theta + p_-^2 \tan^2 \theta,
\]
\[
K_{33}(\theta) = 1 + 2p_- (M_{22} M_{33} + M_{23} M_{32}) \cosh 2h \tan \theta + p_-^2 \tan^2 \theta,
\]
\[
K_{23}(\theta) = 4p_- M_{22} M_{23} \cosh 2h \tan \theta,
\]
\[
K_{32}(\theta) = -4p_- M_{32} M_{33} \cosh 2h \tan \theta.
\]

(6.8)

Now \(K^{(b)}_-(\theta; p_-, M_{\text{spin}})\) does not depend on the submatrix \(M_{\text{charge}}\). Because of the relation

\[
M_{22} M_{33} + M_{23} M_{32} = (1 + 4M_{22} M_{23} M_{32} M_{33})^{\frac{1}{2}},
\]

(6.9)

the solution (6.8) depends on three arbitrary parameters,

\[
p_-, \quad \alpha = M_{22} M_{23}, \quad \beta = -M_{32} M_{33}.
\]

(6.10)

The corresponding boundary term is

\[
-p_- \left\{ (M_{22} M_{33} + M_{23} M_{32}) (n_{\uparrow} - n_{\downarrow}) + 2iM_{22} M_{23} c_{1\uparrow}^\dagger c_{1\downarrow} + 2iM_{32} M_{33} c_{1\downarrow}^\dagger c_{1\uparrow} \right\}
\]

\[
= -p_- \left\{ (1 - 4\alpha \beta) \frac{1}{2} (n_{\uparrow} - n_{\downarrow}) + 2i\alpha c_{1\uparrow}^\dagger c_{1\downarrow} - 2i\beta c_{1\downarrow}^\dagger c_{1\uparrow} \right\}.
\]

(6.11)

This time we see the terms \(c_{1\uparrow}^\dagger c_{1\downarrow}\) and \(c_{1\downarrow}^\dagger c_{1\uparrow}\) which flip the spin of an electron at the boundary site. If we assume \(M_{\text{spin}} \in SU(2)\) (cf. (3.16)), then \(\beta = \alpha^*\) and the boundary term (6.11) becomes hermitian.

The obtained results can be explained by considering the \(SO(4)\) rotation at the boundary site \(m = 1\),

\[
\begin{pmatrix}
\tilde{c}_{1\uparrow}^\dagger & i\tilde{c}_{1\uparrow}^\dagger \\
\tilde{c}_{1\downarrow}^\dagger & i\tilde{c}_{1\downarrow}^\dagger
\end{pmatrix} = M_{\text{spin}}^{-1}
\begin{pmatrix}
c_{1\uparrow}^\dagger & i\tilde{c}_{1\uparrow}^\dagger \\
c_{1\downarrow}^\dagger & i\tilde{c}_{1\downarrow}^\dagger
\end{pmatrix}
\]

(6.12)

where we assume \(M_{\text{charge}}, M_{\text{spin}} \in SU(2)\). The transformation (6.12) changes the boundary chemical potential into

\[
\tilde{n}_{\uparrow} + \tilde{n}_{\downarrow} - 1 = \left( |M_{11}|^2 - |M_{14}|^2 \right) (n_{\uparrow} + n_{\downarrow}) - 2iM_{11} M_{14} c_{1\uparrow}^\dagger c_{1\downarrow} + 2iM_{11}^* M_{14}^* c_{1\downarrow}^\dagger c_{1\uparrow},
\]

(6.13)

while the boundary magnetic field is changed into

\[
\tilde{n}_{\uparrow} - \tilde{n}_{\downarrow} = \left( |M_{22}|^2 - |M_{23}|^2 \right) (n_{\uparrow} + n_{\downarrow}) + 2iM_{22} M_{23} c_{1\uparrow}^\dagger c_{1\downarrow} - 2iM_{22}^* M_{23}^* c_{1\downarrow}^\dagger c_{1\uparrow}.
\]

(6.14)

We see that (6.13) and (6.14) coincide (6.3) and (6.11) respectively. One may check that the Coulomb interaction term is invariant under the transformation (6.12),

\[
\left( \tilde{n}_{\uparrow} - \frac{1}{2} \right) \left( \tilde{n}_{\downarrow} - \frac{1}{2} \right) = \left( n_{\uparrow} - \frac{1}{2} \right) \left( n_{\downarrow} - \frac{1}{2} \right)
\]

(6.15)

as it should be.

Thus we have obtained two non-diagonal solutions of the graded RE (4.4). We have confirmed that under the condition (4.4), the solutions (6.2) and (6.8) provide the most general
solutions of the graded RE (4.3). It is also possible to construct the non-diagonal solutions of the conjugated graded RE (4.7) in a similar way.

Next we clarify the relationship between the two solutions $K^a(\theta; P, M_{\text{charge}})$ (6.1) and $K^b(\theta; P, M_{\text{spin}})$ (6.7). Applying the partial particle-hole transformation of the fermionic $R$-matrix to the graded RE (1.5), we find that for a given solution $K^a(\theta, h(\theta))$,

$$K^a(\theta, h(\theta)) = QK^a(\theta, -h(\theta))Q^{-1}. \tag{6.16}$$

is also a solution of the graded RE (1.3). Here we have explicitly written the parameter $h(\theta)$. The transformation $h(\theta) \rightarrow -h(\theta)$ corresponds to $U \rightarrow -U$. Then the solution (6.7) is connected with the solution (6.1) through the following formula,

$$K^b(\theta, h(\theta); P, M_{\text{spin}}) = QK^a(\theta, -h(\theta); P, M_{\text{charge}})Q^{-1}. \tag{6.17}$$

Here the matrix elements of $M_{\text{charge}}$ are exchanged with those of $M_{\text{spin}}$. In fact one can see that the partial particle-hole transformation (1.9) changes the boundary term (6.5) into (6.11) with the exchange $M_{\text{charge}} \leftrightarrow M_{\text{spin}}$.

§7. Conclusion

In this paper we have studied the integrable boundary conditions for the 1D Hubbard model from the point of view of the Quantum Inverse Scattering Method. We have treated both the twisted periodic boundary condition and the open boundary condition. The most important object in the investigation is the fermionic $R$-matrix for the 1D Hubbard model found by Olmedilla et al. [22]. It has an interesting symmetry matrix, which reflects the $SO(4)$ symmetry of the Hamiltonian. Using the symmetry matrix, we have found the general twisted periodic boundary condition. In a sense, the periodic boundary condition can be twisted by applying the $SO(4)$ rotation to the boundary operators. We have also found the discrete symmetry of the fermionic $R$-matrix, which corresponds to the partial particle-hole transformation for the Hamiltonian. Recently the $SO(4)$ symmetry of the transfer matrix was investigated by Göhmann and Murakami [32]. The symmetry of the fermionic $R$-matrix is directly connected with the $SO(4)$ symmetry of the transfer matrix [31].

For the integrable open boundary conditions, we have formulated the graded reflection equation in terms of the fermionic $R$-matrix. By solving directly the functional equations, we have obtained the diagonal $K$-matrices. There are two types of the $K$-matrices, which correspond to a) the boundary chemical potential and b) the boundary magnetic field. Moreover we have obtained non-diagonal $K$-matrices using the covariance property of the graded reflection equation. We can rotate the diagonal boundary fields by means of the $SO(4)$ symmetry. The two types of solutions are related through a partial particle-hole transformation for the fermionic $R$-matrix.

Recently there was reported some important progress in the evaluation of the eigenvalues of the transfer matrices of the 1D Hubbard model [35, 36]. It is an interesting problem to generalize these results to the model with the twisted periodic boundary conditions and the open boundary condition.
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Appendix: Diagonal Solutions of the Graded Reflection Equation

We solve the graded RE (5.2) for the diagonal $K_-(\theta)$

\[ R_{12}(\theta_1, \theta_2) K_-(\theta_1) R_{12}^*(\theta_1, -\theta_2) K_-(\theta_2) = K_-(\theta_2) R_{12}(\theta_1, -\theta_2) K_-(\theta_1) R_{12}^*(\theta_1, \theta_2). \]  

(A.1)

Let us introduce the Boltzmann weights of $R_{12}(\theta_1, -\theta_2)$

\[ R_{12}(\theta_1, -\theta_2) = \begin{pmatrix}
\tilde{a}_+ & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -i\tilde{b}_+ & 0 & 0 & \tilde{c} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -i\tilde{b}_+ & 0 & 0 & 0 & 0 & 0 & \tilde{c} & 0 \\
0 & 0 & 0 & -\tilde{c}^+ & 0 & 0 & 0 & -i\tilde{f} & 0 & 0 \\
0 & \tilde{c} & 0 & 0 & i\tilde{b}^- & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -\tilde{a}^- & 0 & 0 & 0 & 0 \\
0 & 0 & i\tilde{f} & 0 & 0 & \tilde{c}^- & 0 & 0 & -\tilde{d}^- & 0 \\
0 & 0 & 0 & 0 & i\tilde{b}^- & 0 & 0 & 0 & 0 & \tilde{c} \\
0 & 0 & \tilde{c} & 0 & 0 & 0 & 0 & 0 & -\tilde{a}^- & 0 \\
0 & 0 & 0 & -i\tilde{f} & 0 & 0 & -\tilde{d}^- & 0 & 0 & \tilde{c}^- & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -\tilde{a}^- & 0 & 0 & \tilde{c}^- & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -i\tilde{f} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\tilde{c}^+ & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \tilde{c} & 0 & 0 & -\tilde{c}^+ & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\tilde{b}^+ & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \tilde{c} & 0 & -\tilde{b}^+ & 0 \\
\end{pmatrix} \]

(A.2)

where

\[ \tilde{a}^\pm = \cos^2(\theta_1 + \theta_2) \left\{ 1 \pm \tanh(h_1 + h_2) \frac{\cos(\theta_1 - \theta_2)}{\cos(\theta_1 + \theta_2)} \right\}, \]

\[ \tilde{b}^\pm = \sin(\theta_1 + \theta_2) \cos(\theta_1 + \theta_2) \left\{ 1 \pm \tanh(h_1 + h_2) \frac{\sin(\theta_1 - \theta_2)}{\sin(\theta_1 + \theta_2)} \right\}, \]

\[ \tilde{c}^\pm = \sin^2(\theta_1 + \theta_2) \left\{ 1 \pm \tanh(h_1 - h_2) \frac{\sin(\theta_1 - \theta_2)}{\sin(\theta_1 + \theta_2)} \right\}, \]

\[ \tilde{d}^\pm = 1 \pm \tanh(h_1 + h_2) \frac{\cos(\theta_1 + \theta_2)}{\cos(\theta_1 - \theta_2)}, \]

\[ \tilde{c} = \frac{\cos(\theta_1 + \theta_2)}{\cosh(h_1 + h_2)}, \quad \tilde{f} = \frac{\sin(\theta_1 + \theta_2)}{\cosh(h_1 - h_2)} \]  

(A.3)
We note useful relations among the Boltzmann weights of $R$-matrix,

\[
\begin{align*}
\frac{a^\pm}{e} &= e^{\pm(h_1-h_2)} \cos \theta_1 \cos \theta_2 + e^{\mp(h_1-h_2)} \sin \theta_1 \sin \theta_2, \\
\frac{c^\pm}{f} &= e^{\pm(h_1+h_2)} \sin \theta_1 \cos \theta_2 - e^{\mp(h_1+h_2)} \cos \theta_1 \sin \theta_2, \\
\frac{\tilde{a}^\pm}{\tilde{e}} &= e^{\pm(h_1+h_2)} \cos \theta_1 \cos \theta_2 - e^{\mp(h_1+h_2)} \sin \theta_1 \sin \theta_2, \\
\frac{\tilde{c}^\pm}{f} &= e^{\pm(h_1-h_2)} \sin \theta_1 \cos \theta_2 + e^{\mp(h_1-h_2)} \cos \theta_1 \sin \theta_2,
\end{align*}
\]

The graded RE (A.1) for the diagonal $K_-(\theta)$ is equivalent to the following set of 10 equations:

\[
\begin{align*}
\frac{b^\pm}{e} &= e^{\pm(h_1-h_2)} \sin \theta_1 \cos \theta_2 - e^{\pm(h_1-h_2)} \cos \theta_1 \sin \theta_2 = \sin(\theta_1 - \theta_2) \sin(\theta_1 + \theta_2) \frac{\tilde{d}^\pm}{f}, \\
\frac{b^\pm}{f} &= e^{\pm(h_1+h_2)} \cos \theta_1 \cos \theta_2 + e^{\pm(h_1+h_2)} \sin \theta_1 \sin \theta_2 = \cos(\theta_1 - \theta_2) \cos(\theta_1 + \theta_2) \frac{\tilde{d}^\pm}{e}, \\
\frac{\tilde{b}^\pm}{e} &= e^{\pm(h_1+h_2)} \sin \theta_1 \cos \theta_2 + e^{\pm(h_1+h_2)} \cos \theta_1 \sin \theta_2 = \sin(\theta_1 - \theta_2) \sin(\theta_1 + \theta_2) \frac{\tilde{d}^\pm}{f}, \\
\frac{\tilde{b}^\pm}{f} &= e^{\pm(h_1-h_2)} \cos \theta_1 \cos \theta_2 - e^{\pm(h_1-h_2)} \sin \theta_1 \sin \theta_2 = \cos(\theta_1 - \theta_2) \cos(\theta_1 + \theta_2) \frac{\tilde{d}^\pm}{e}.
\end{align*}
\]

(A.4)

(A.5)
where $\alpha$ We shall solve the functional equations (A.5)–(A.10) and (A.15)–(A.18). First, let us consider

From (A.19), we get

Due to the relations (A.4), the functional equations (A.11)–(A.14) reduce to

Due to the relations (A.4), the functional equations (A.11)–(A.14) reduce to

We shall solve the functional equations (A.5)–(A.10) and (A.15)–(A.18). First, let us consider

Using (A.4), we find that (A.3) is equivalent to

From (A.19), we get

where $\alpha$ is a constant. Similarly, from (A.6)–(A.8), we get

(20)

(21)

(22)

(23)
where \( \alpha_i \) (\( i = 2, 3, 4 \)) are constants. Now from (A.15) we have

\[
\cot \theta_2 \frac{e^{h_2} x_2(\theta_2)}{x_1(\theta_2)} - e^{-h_2} = \cot \theta_1 \frac{e^{-h_1} - e^{h_1} x_3(\theta_1)}{x_1(\theta_1)}.
\]

(A.24)

Substituting (A.20) and (A.23) into (A.24), we find a constraint between the constants

\[ \alpha_1 = -\alpha_4. \]

(A.25)

Similarly, from (A.16), we find

\[ \alpha_2 = -\alpha_3. \]

(A.26)

Equations (A.17) and (A.18) give the constraints (A.26) and (A.25) respectively. Finally let us consider a consistency condition

\[
\frac{x_2(\theta) x_4(\theta)}{x_1(\theta) x_2(\theta)} = \frac{x_3(\theta) x_4(\theta)}{x_1(\theta) x_3(\theta)}.
\]

(A.27)

With the constraints (A.25) and (A.26), (A.27) gives a relation

\[
\frac{e^{-h} + \alpha_1 e^h \tan \theta}{e^h - \alpha_1 e^{-h} \tan \theta} = \frac{e^{-h} + \alpha_2 e^h \tan \theta}{e^h - \alpha_2 e^{-h} \tan \theta},
\]

from which we find

\[ \alpha_1 = \pm \alpha_2. \]

(A.29)

Thus there are two possibilities for \( x_i(\theta) \) (\( i = 1, \ldots, 4 \)).

a) \( \alpha_1 = \alpha_2 = -\alpha_3 = -\alpha_4 = \alpha \)

\[
\frac{x_2(\theta)}{x_1(\theta)} = \frac{e^{-h} + \alpha e^h \tan \theta}{e^h - \alpha e^{-h} \tan \theta}, \quad \frac{x_3(\theta)}{x_1(\theta)} = \frac{e^{-h} + \alpha e^h \tan \theta}{e^h - \alpha e^{-h} \tan \theta},
\]

(A.30)

b) \( \alpha_1 = -\alpha_2 = \alpha_3 = -\alpha_4 = \alpha \)

\[
\frac{x_2(\theta)}{x_1(\theta)} = \frac{e^{-h} + \alpha e^h \tan \theta}{e^h - \alpha e^{-h} \tan \theta}, \quad \frac{x_3(\theta)}{x_1(\theta)} = \frac{e^{-h} - \alpha e^h \tan \theta}{e^h + \alpha e^{-h} \tan \theta},
\]

(A.31)

Here \( \alpha \) is an arbitrary constant. It is easy to confirm that both cases (A.30) and (A.31) satisfy the remaining functional equations (A.9) and (A.10). To conclude, we have shown that there are two diagonal solutions of the RE (A.1). The solutions (A.30) and (A.31) are equivalent to (5.5) and (5.6), respectively.
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