Fermionic $R$-operator approach for the small-polaron model with open boundary condition

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Exact integrability and algebraic Bethe ansatz of the small-polaron model with the open boundary condition are discussed in the framework of the quantum inverse scattering method (QISM). We employ a new approach where the fermionic $R$-operator which consists of fermion operators is a key object. It satisfies the Yang-Baxter equation and the reflection equation with its corresponding $K$-operator. Two kinds of 'super-transposition' for the fermion operators are defined and the dual reflection equation is obtained. These equations prove the integrability and the Bethe ansatz equation which agrees with the one obtained from the graded Yang-Baxter equation and the graded reflection equations.

1 Introduction

There have been reported various one-dimensional (1D) integrable models. In 1D systems, some physical properties are beyond the perturbative interpretation [1] and therefore integrable models have attracted much interest. Among the integrable fermion models, the simplest but non-trivial one is the small-polaron model, a spinless fermion model with a hopping term and an interaction term. It describes the motion of an additional electron in a polar crystal [2] and exhibits some properties that differ from those of the Fermi liquid.

The integrability and other properties for the small-polaron model with open boundary condition have been studied in many ways. By use of the coordinate Bethe ansatz and the string hypothesis the critical value of attractive boundary potential for a boundary bound state was shown. [3] In the quantum inverse scattering method (QISM), the integrability and the Bethe ansatz equation were derived from the graded Yang-Baxter equation and the graded reflection equations. [4, 5, 6]

In the QISM, the graded Yang-Baxter equation plays an important role for the fermion models. The corresponding spin models through the Jordan Wigner transformation are
often useful. Using the correspondence, we obtain the graded Yang-Baxter equation from
the Yang-Baxter equation of the spin model. There, the graded Grassmann product
and the super-trace are introduced. We know that the small-polaron model is related with
the \(XXZ\) Heisenberg model.

Recently we introduced a fermionic \(R\)-operator. It clarifies the integrable structure of
the fermion models with the periodic boundary condition. The fermionic \(R\)-operator satisfies
the Yang-Baxter equation. The 'super-trace' of the fermion operator is introduced and
the commutativity of the transfer operator proves the integrability. Furthermore
this fermionic \(R\)-operator enables us to evaluate thermodynamic quantities for the fermion
system through the quantum transfer matrix (QTM) method. In the QTM method, partition
function is estimated in two dimensional space (the quantum space and the auxiliary
space). The transfer operator exhibits the integrable structure and the QTM leads to the
partition function. The former operates on the quantum space, on the other hand, the
latter operates on the auxiliary space. Because the fermionic \(R\)-operator has the same
footing on both spaces, the QTM method can be applied.

In this paper we extend the fermionic \(R\)-operator approach to the open boundary
condition. In §2, we briefly review the periodic boundary case of the small-polaron model
with this \(R\)-operator approach, where 'super-trace' (Str) is introduced. The Yang Baxter
equation leads to the integrability and the Bethe ansatz equation. We also investigate the
properties of the fermionic \(R\)-operator and define two kinds of 'super-transposition' (st
and st). In §3, we prove the integrability with the open boundary condition. We obtain
the reflection equation and the dual reflection equation and prove the commutativity of
the transfer operator. In §4, we evaluate the eigenvalue of the transfer operator and get
the corresponding Bethe ansatz equation. This result agrees with the one obtained by the
graded Yang Baxter approach. The last section is devoted to the concluding remarks.

2 \textbf{Small-polaron model with periodic boundary condition}

We summarize the fermionic \(R\)-operator approach to the small-polaron model with the
periodic boundary condition. The Hamiltonian of this system is

\[
H = \sum_{j=1}^{N} H_{jj+1},
\]

\[
H_{jj+1} = -t \{c_{j+1}^{\dagger} c_j + c_j^{\dagger} c_{j+1}\} + V n_j n_{j+1},
\]

where \(t\) represents the overlapping integral and \(V\) the electron-phonon coupling. The fermionic \(R\)-operator,

\[
R_{ab}(u) = a(u) \{\{-n_an_b + \bar{n}_a\bar{n}_b\}\} + b(u) \{n_an_b + \bar{n}_a\bar{n}_b\} + c(u) \{c_a^{\dagger} c_b + c_b^{\dagger} c_a\},
\]

\[
a(u) = \frac{\sin(u + 2\eta)}{\sin 2\eta}, \quad b(u) = \frac{\sin u}{\sin 2\eta}, \quad c(u) = 1,
\]
consists of fermion operators where \( n_a = c_a^\dagger c_a \) and \( \bar{n}_a = 1 - n_a \). This \( R \)-operator satisfies the Yang Baxter equation,

\[
R_{12}(u-v)R_{13}(u)R_{23}(v) = R_{23}(v)R_{13}(u)R_{12}(u-v).
\] (5)

As is the routine for the quantum inverse scattering method, from the equation (5) we have the global Yang Baxter equation,

\[
R_{ab}(u-v)T_a(u)T_b(v) = T_b(v)T_a(u)R_{ab}(u-v),
\] (6)

where the monodromy operator is expressed by

\[
T_a(u) = R_{aN} \ldots R_{a1}
\] (7)

\[
= A(u)\bar{n}_a + B(u)c_a + C(u)c_a^\dagger + D(u)n_a.
\] (8)

Here the suffix 1, 2, \ldots \( N \) mean the quantum space and the suffix \( a, b \) the auxiliary space. This equation (6) leads to the commutativity of the transfer operators \( \tau(u) \),

\[
[\tau(u), \tau(v)] = 0,
\] (9)

\[
\tau(u) = \text{Str}_a T_a(u) = A(u) - D(u).
\] (10)

Here 'super-trace' for the fermion operators (Str) is defined as

\[
\text{Str}_a X_a = a \langle 0|X_a|0\rangle_a - a \langle 1|X_a|1\rangle_a,
\] (11)

where \( |0\rangle_a \) and \( |1\rangle_a \) are the fermion Fock states satisfying \( |1\rangle_a = c_a^\dagger|0\rangle_a \) and \( |0\rangle_a = c_a|1\rangle_a \). This means that the system has a sufficient number of conserved operators and therefore is integrable. The logarithmic derivative of the transfer operator at \( u = 0 \) gives the Hamiltonian defined by (1) and (2) with

\[
t = -\frac{1}{\sin 2\eta}, \quad V = \frac{\cos 2\eta}{\sin 2\eta}.
\] (12)

The energy spectrum is obtained from the eigenvalue of the transfer operator. The eigenstate \( |\phi\rangle \) and the eigenvalue \( \Lambda(u) \) of the transfer operator are given by

\[
\tau(u)|\phi\rangle = \Lambda(u)|\phi\rangle, \quad |\phi\rangle = \prod_{j=1}^M B(u_j)|0\rangle,
\] (13)

\[
\Lambda(u) = a(u)^N \prod_{j=1}^M a(u_j - u) - b(u)^N \prod_{j=1}^M \frac{a(u - u_j)}{b(u - u_j)},
\] (14)

where \( |0\rangle \) is a pseudovacuum state. There is a constraint on \( u_j (j = 1 \ldots M) \) (the Bethe ansatz equation) so that (13) should be satisfied,

\[
\left( \frac{a(u_i)}{b(u_i)} \right)^N = \prod_{j\neq i, j=1}^M \frac{a(u_i - u_j)}{a(u_j - u_i)}.
\] (15)
In terms of the solution \( \{u_j\} \) of (15), the energy spectrum is given by

\[
E = \frac{d}{du} \log \Lambda(u)|_{u=0} = N \cot 2\eta - \sum_{j=1}^{M} \frac{\sin 2\eta}{\sin u_j \sin (u_j + 2\eta)}.
\] (16)

The fermionic \( R \)-operator has important properties which are useful further in the analysis. We define two kinds of ‘super-transposition’ for the fermion operators (st and \( \bar{st} \)) so that \((X_{a}^{st})^{st} = X_{a}\) for any fermion operator \( X \),

\[
X_{a} = A\tilde{n}_{a} + Bc_{a} + Cc_{a}^{\dagger} + Dn_{a},
\] (17)

\[
X_{a}^{st} = A\tilde{n}_{a} + Bc_{a}^{\dagger} + Cc_{a} + Dn_{a},
\] (18)

\[
X_{a}^{\bar{st}} = A\tilde{n}_{a} - Bc_{a}^{\dagger} + Cc_{a} + Dn_{a}.
\] (19)

The unitarity and the crossing unitarity conditions are satisfied as follows,

**Unitarity**

\[
R_{12}(u)R_{12}(-u) = \rho(u), \quad \rho(u) = 1 - \frac{\sin^2 u}{\sin^2 2\eta}.
\] (20)

**Crossing unitarity**

\[
R_{12}(u)^{st}R_{12}(-u - 4\eta)^{st} = \tilde{\rho}(u), \quad \tilde{\rho}(u) = 1 - \frac{\sin^2(u + 2\eta)}{\sin^2 2\eta}.
\] (21)

We also have a property,

\[
R_{12}(u)^{st} = R_{12}(u)^{st}. \quad (22)
\]

In the next section, we shall discuss the fermionic \( R \)-operator approach for the open boundary condition.

### 3 Exact integrability with open boundary condition

To treat the open boundary condition, we consider the Yang-Baxter equation and the reflection equations. For the fermionic \( R \)-operator given by (3), we look for the fermionic \( K \)-operator which satisfies the reflection equation,

\[
R_{12}(u - v)K_{1}(u)R_{12}(u + v)K_{2}(v) = K_{2}(v)R_{12}(u + v)K_{1}(u)R_{12}(u - v).
\] (23)

We find that the fermionic \( K \)-operator is given by

\[
K_a(u) = -\frac{\sin(u - t)}{\sin t}n_a + \frac{\sin(u + t)}{\sin t}\tilde{n}_a.
\] (24)
We have a more general form of the fermionic $K$-operator, but we here restrict the $K$-operator to be even operator. Then the global reflection equation,

$$R_{ab}(u - v)\mathcal{T}_a(u)R_{ab}(u + v)\mathcal{T}_a(v) = \mathcal{T}_b(v)R_{ab}(u + v)\mathcal{T}_a(u)R_{ab}(u - v),$$  \hspace{1cm} (25)$$

is satisfied where the double monodromy operator is

$$\mathcal{T}_a(u) = T_a(u)K_a(u)T_a^{-1}(-u).$$  \hspace{1cm} (26)$$

We also show the dual reflection equation,

$$\bar{R}_{12}(-u_+)K^+_1(u)^{st_1}R_{12}(-u_+ - 4\eta)K^+_2(v)^{st_2} = K^+_2(v)^{st_2}R_{12}(-u_+ - 4\eta)K^+_1(u)^{st_1}R_{12}(-u_-),$$  \hspace{1cm} (27)$$

where $\bar{R}_{ab}(u) = R_{ab}(u)^{st_a\bar{st}_b}$ and $u_{\pm} = u \pm v$. This dual reflection equation (27) will be used for a proof of the commutativity of the transfer operator. The dual $K$-operator is found to be

$$K^+_a(u) = \sin(u + 2\eta - t^+)\bar{n}_a + \sin(u + 2\eta + t^+)n_a.$$  \hspace{1cm} (28)$$

Next we prove the commutativity of the transfer operators with different spectral parameters. We define the transfer operator as

$$t(u) = \text{Str}_a \{ K^+_a(u)\mathcal{T}_a(u) \}. \hspace{1cm} (29)$$

We prepare some properties of the 'super-trace' and the 'super-transposition' for the fermion operators. When $Y$ is an even fermion operator and $X$ operates trivially except on $a$ space, we have

$$\{ X_a Y_{ab} \}^{st_a} = Y_{ab}^{st_a} X_a^{st_a}. \hspace{1cm} (30)$$

When $X$ and $Y$ are even fermion operators, we have

$$\text{Str}_{ab} \{ X_a Y_{ab} \} = \text{Str}_{ab} \{ X_{ab}^{st_a} Y_{ab}^{st_a} \}. \hspace{1cm} (31)$$

When $X$ and $Y$ are even fermion operators and $X$ operates trivially except on $a$ and $b$ spaces, we have

$$\{ X_{ab} Y_{ab} \}^{st_a \bar{st}_b} = Y_{ab}^{st_a \bar{st}_b} X_{ab}^{st_a \bar{st}_b}, \hspace{1cm} (32)$$

$$\text{Str}_{ab} \{ X_{ab} Y_{ab} \} = \text{Str}_{ab} \{ Y_{ab} X_{ab} \}. \hspace{1cm} (33)$$

The relation $t(u)t(v) = t(v)t(u)$ is to be proved. We begin with

$$t(u)t(v) \hspace{1cm} (34)$$

$$= \text{Str}_a \{ K^+_a(u)\mathcal{T}_a(u) \} \text{Str}_b \{ K^+_b(v)\mathcal{T}_b(v) \} \hspace{1cm} (35)$$

$$= \text{Str}_a \{ K^+_a(u)^{st_a} \mathcal{T}_a(u)^{st_a} \} \text{Str}_b \{ K^+_b(v)^{st_b} \mathcal{T}_b(v)^{st_b} \} \hspace{1cm} (36)$$

$$= \text{Str}_{ab} [ K^+_a(u)^{st_a} \mathcal{T}_a(u)^{st_a} K^+_b(v)^{st_b} \mathcal{T}_b(v)^{st_b} ] \hspace{1cm} (37)$$
Because $K$-operator is even, $\mathcal{T}_a(u)^{\text{sta}}$ commutes with $K_b^+(v)$. From the crossing unitarity (21), the identity operator can be inserted as

$$
\rho^{-1}_+ \text{Str}_ab\{K_a^+(u)^{\text{sta}}K_b^+(v)R_{ab}(-u_+ - 4\eta)\}^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v) = \rho^{-1}_+ \text{Str}_ab\{K_a^+(u)^{\text{sta}}R_{ab}(-u_+ - 4\eta)K_b^+(v)\}^{\text{sta}}R_{ab}(u_+)\mathcal{T}_b(v)\}^{\text{sta}}
$$

(38)

$$
= \rho^{-1}_+ \text{Str}_ab\{K_a^+(u)^{\text{sta}}R_{ab}(-u_+ - 4\eta)K_b^+(v)\}^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)
$$

(39)

$$
= \rho^{-1}_+ \text{Str}_ab\{K_a^+(u)^{\text{sta}}R_{ab}(-u_+ - 4\eta)K_b^+(v)\}^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)
$$

(40)

The above equalities are due to the properties (30) and (31) respectively, where $u_\pm = u \pm v, \rho_\pm = \rho(u_\pm), \tilde{\rho}_\pm = \tilde{\rho}(u_\pm)$.

Then from the unitarity (20) and property (32), we get

$$
\rho^{-1}_+ \text{Str}_ab\{R_{ab}(-u_-)^{\text{sta}t}K_a^+(u)^{\text{sta}}R_{ab}(-u_+ - 4\eta)K_b^+(v)\}^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)
$$

(41)

$$
= \rho^{-1}_+ \text{Str}_ab\{R_{ab}(u_-)^{\text{sta}}K_a^+(u)^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)\}
$$

(42)

Here the reflection equation (23) and the dual reflection equation (27) can be applied,

$$
\rho^{-1}_+ \text{Str}_ab\{R_{ab}(u_-)^{\text{sta}}K_b^+(v)^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)\}
$$

(43)

$$
= \rho^{-1}_+ \text{Str}_ab\{R_{ab}(u_-)^{\text{sta}}K_a^+(u)^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)\}
$$

(44)

For this expression, we do the other way around. The property (32) is used in the above, and the property (33) and then the use of the unitarity (20) give

$$
\rho^{-1}_+ \text{Str}_ab\{R_{ab}(u_-)^{\text{sta}}K_b^+(v)^{\text{sta}}R_{ab}(u_+)\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)\}
$$

(45)

$$
= \rho^{-1}_+ \text{Str}_ab\{K_b^+(v)^{\text{sta}}R_{ab}(u_-)^{\text{sta}t}K_a^+(u)\}^{\text{sta}}\mathcal{T}_b(v)\}^{\text{sta}}\mathcal{T}_a(u)^{\text{sta}}\mathcal{T}_b(v)
$$

(46)

Thus, the commutativity of transfer operator is proved.

We relate the transfer operator $t(u)$ to the Hamiltonian of this system. The derivative of the transfer operator is considered. We have $K_a(0) = 1, \mathcal{T}_a(0) = 1$ and

$$
t(0) = \text{Str}_a K_a^+(0) = -2 \cos 2\eta \sin t^+.
$$

(47)

Using these relations, we obtain

$$
t'(0) = \text{Str}_a K_a^{+(0)} + \text{Str}\{K_a^+(0)R'_{aN}(0)P_{aN}\} + \text{Str} K_a^{+(0)} \sum_{j=1}^{N-1} R'_{j+1j}(0)P_{j+1j}
$$

$$
+ \text{Str}_a K_a^+(0)K_1^+(0) + \text{Str}_a K_a^{+(0)} \sum_{j=1}^{N-1} P_{j+1j}R'_{j+1j}(0) + \text{Str}_a \{K_a^+(0)P_{aN}R'_{aN}(0)\}
$$

(48)
Here ’ means the derivative with respect to $u$. The Hamiltonian density $H_{jj+1}$, (2) with (12), is expressed as $H_{jj+1} = R'_{j+1j}(0)P_{j+1j} = P_{j+1j}R'_{j+1j}(0)$. Thus the Hamiltonian is given by

$$H = \frac{1}{2}t(0)^{-1}(t'(0) - \text{Str}_a K^+_a(0))$$

$$= \sum_{j=1}^{N-1} H_{jj+1} - \frac{1}{2} \cot t(2n_1 - 1) + \frac{1}{2} \cot t^+(2n_N - 1)$$

(49) (50)

4 Algebraic Bethe ansatz

In this section, the eigenvalue and the eigenstate of the transfer operator are discussed. The double monodromy operator (26) is expressed by

$$\mathcal{T}_a(u) = \mathcal{A}(u)\bar{n}_a + \mathcal{B}(u)c_a + \mathcal{C}(u)c^+_a + \mathcal{D}(u)n_a.$$  

(51)

Because the double-monodromy operator is an even operator, $\mathcal{B}(u)$ should have the property of the creation operator. We construct the eigenvector algebraically. We introduce the eigenvector of the transfer operator by

$$|\Phi\rangle = \prod_{j=1}^{M} \mathcal{B}(u_j)|0\rangle.$$  

(52)

The double-monodromy operator (51) is also expressed with the monodromy operators (8),

$$\mathcal{T}_a(u) = T_a(u)K_a(u)T_a^{-1}(-u),$$

$$T_a(u) = A(u)\bar{n}_a + B(u)c_a + C(u)c^+_a + D(u)n_a,$$

$$T_a^{-1}(u) = \bar{A}(u)\bar{n}_a + \bar{B}(u)c_a + \bar{C}(u)c^+_a + \bar{D}(u)n_a.$$  

(53) (54) (55)

The above relations give $\mathcal{A}(u)\ldots\mathcal{D}(u)$ in terms of $\mathcal{A}(u)\ldots\mathcal{D}(u)$ and $\bar{A}(u)\ldots\bar{D}(u)$. We have the relations between $\mathcal{A}(u)\ldots\mathcal{D}(u)$ and $\bar{A}(u)\ldots\bar{D}(u)$ obtained from the global Yang Baxter equation (6) with $v = -u$

$$T_b^{-1}(-u)R_{ab}(2u)T_a(u) = T_a(u)R_{ab}(2u)T_b^{-1}(-u).$$

(56)

It is convenient to use $\tilde{\mathcal{D}}(u)$,

$$\tilde{\mathcal{D}}(u) = \sin(2u + 2\eta)\mathcal{D}(u) - \sin 2\eta \mathcal{A}(u)$$

instead of $\mathcal{D}(u)$. The eigenvalue of $\tilde{\mathcal{D}}(u)$ acting on the pseudovacuum $|0\rangle$ takes a simpler form than that of $\mathcal{D}(u)$,

$$\mathcal{A}(u)|0\rangle = \frac{\sin(u + t)}{\sin t}a(u)^{2N}|0\rangle,$$

$$\tilde{\mathcal{D}}(u)|0\rangle = -\frac{\sin 2u \sin(u + 2\eta - t)}{\sin t}b(u)^{2N}|0\rangle.$$  

(58) (59)
we have

From the relation (49), the energy spectrum is

\[ \Lambda(u) = -\frac{\sin(2u + 4\eta) \sin(u - t^+) \sin(u + t)}{\sin(2u + 2\eta)} a(u)^2 \prod_{j=1}^{M} \frac{\sin(u - u_j - 2\eta) \sin(u + u_j)}{\sin(u - u_j) \sin(u + u_j + 2\eta)} \]

\[ -\frac{\sin(u + 2\eta + t^+) \sin(u + 2\eta - t)}{\sin(2u + 2\eta)} b(u)^2 \prod_{j=1}^{M} \frac{\sin(u + u_j + 4\eta) \sin(u - u_j + 2\eta)}{\sin(u - u_j) \sin(u + u_j + 2\eta)} , \]

and the Bethe ansatz equations \( l = 1, \ldots, M \),

\[ \left\{ \frac{a(u_j)}{b(u_l)} \right\}^{2N} = \frac{\sin(u_l + 2\eta + t^+) \sin(u_l + 2\eta - t)}{\sin(u_l - t^+) \sin(u_l + t)} \prod_{j \neq l, j=1}^{M} \frac{\sin(u_l + u_j + 4\eta) \sin(u_l - u_j + 2\eta)}{\sin(u_l - u_j - 2\eta) \sin(u_l + u_j)} . \]

From the relation \([49]\), the energy spectrum is

\[ E = -(N - 1) \cot 2\eta - \frac{1}{2} \cot t + \frac{1}{2} \cot t^+ + \frac{1}{\sin 4\eta} - 2 \sum_{j=1}^{M} \frac{\sin 2\eta}{\sin u_j \sin(u_j + 2\eta)} . \]
5 Concluding Remarks

In this paper, we have extended the fermionic $R$-operator approach for the small polaron model with the open boundary condition. The Yang-Baxter equation and the reflection equations are satisfied among the fermionic $R$-operators and the fermionic $K$-operators which consist of fermion operators. The properties of the fermionic $R$-operators and the 'super-trace' and the 'super-transposition' for the fermion operators play an important role. This approach gives a simpler and clearer description than the usual graded Yang-Baxter approach. The integrability and the Bethe ansatz equation are obtained in a unified manner.

We discuss future problems related to this work. First, we solve the Bethe ansatz equations numerically to get the physical quantities. Second, we further extend the fermionic $R$-operator approach to the boundary impurity problems. Last but not least, we develop the quantum transfer matrix method for open boundary condition. We note that this problem remains to be open.

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APPENDIX A: Comparison with the spin system

The small polaron model corresponds to the XXZ Heisenberg model through the Jordan Wigner transformation. For the periodic boundary condition (p.b.c.), the fermion system and the spin system are not exactly the same. The energy spectrum and its Bethe ansatz equation for the fermion system are given by (15) and (16) while those for the spin system are given by

\[ E = \frac{d}{du} \log \Lambda(u)|_{u=0} = N \cot 2\eta - \sum_{j=1}^{M} \frac{\sin 2\eta}{\sin u_j \sin(u_j + 2\eta)}, \quad (A.1) \]

\[ \left( \frac{a(u_i)}{b(u_i)} \right)^N = \prod_{j \neq i, j=1}^{M} \left( -\frac{a(u_i - u_j)}{a(u_j - u_i)} \right). \quad (A.2) \]

We see that the right hand side of (15) and (A.2) are different in signs. It reflects the difference between p.b.c. of fermion system and that of spin system caused by non-locality of the Jordan Wigner transformation.

On the other hand, the small polaron model with open boundary condition is equivalent to the XXZ Heisenberg model with boundary magnetic field and their energy spectrums are exactly the same.
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