Direct Calculation of Thermodynamic Quantities for Heisenberg Model

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Abstract

The XXX Heisenberg model is studied at finite temperature. The free energy is derived without recourse to Thermal Bethe Ansatz method and Quantum Transfer Matrix method. The result perfectly agrees with the free energy derived by Thermal Bethe Ansatz method. An explicit expression of the cluster expansion coefficient in arbitrary order is presented for the first time.

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1 Introduction

In a pioneer work [1], H. Bethe solved the XXX Heisenberg model. The Hamiltonian of the model is written as

\[ H (J, h) = -J \sum_{j=1}^{N} (S_{x}^{x} S_{j+1}^{x} + S_{y}^{y} S_{j+1}^{y} + S_{z}^{z} S_{j+1}^{z}) + 2h \sum_{j=1}^{N} S_{x}^{x} + \text{constant}, \]  

(1.1)

where \( J \) is the coupling constant and \( h \) is the external field. The energy of the system is given by

\[ E_{M} = 2hM + \sum_{j=1}^{M} \frac{2J}{x_{j}^{2} + 1}, \]  

(1.2)

where \( M \) is the number of up-spins and the variables \( x_{j} \) are required to satisfy the Bethe Ansatz (BA) equation,

\[ \left( \frac{x_{j} + i}{x_{j} - i} \right)^{N} = \prod_{j' \neq j} \frac{x_{j} - x_{j'} + 2i}{x_{j} - x_{j'} - 2i}. \]  

(1.3)

It was shown [1] that every eigenstate of this model corresponds to a solution of this simultaneous equation.

The XXX Heisenberg model is the quantum integrable system. Thermal Bethe Ansatz method (TBA) [2] and Quantum Transfer Matrix method (QTM) [3, 4, 5, 6, 7] are the well-known methods to derive thermodynamic quantities for quantum integrable systems. TBA was originated by Yang and Yang [2], who derived the thermodynamics of repulsive \( \delta \)-function boson system. Then, on the assumption of the so-called string hypothesis, M.Takahashi [8] applied TBA to the Heisenberg model. Recently, some analytical results of thermodynamic quantities using QTM were presented by A. Klümper [9, 10]. Many pieces of concept with respect to QTM had been introduced before then. The equivalence of the results using TBA and QTM was proved by several researchers [11, 12, 9, 13].

Our purpose is to derive the free energy of this system independent of TBA and QTM. In this paper, we use a method which we call a direct method. We start from the string hypothesis. There is no other mathematical assumptions except the string hypothesis. In other words, using the direct method, a problem based on the string hypothesis is solved. On the other hand, TBA is a method to solve the problem using a definition of non-equilibrium state entropy. As a main result of this paper, the direct method justifies TBA.
The direct method was used for the $\delta$-function bose system $[14, 15, 16, 17]$. We apply the method to the Heisenberg model here. We define $z$ and $\beta$ as $z \equiv e^{-2\beta h}$ and $\beta \equiv \frac{1}{k_B T}$. The direct method enables us to express the cluster expansion coefficients $b_n$ in arbitrary order explicitly,

$$\log \left[ z^{N/2} \text{Tr} \ e^{-\beta H(J,h)} \right] \equiv \sum_{n=1}^{\infty} b_n z^n, \quad (1.4)$$

and the free energy,

$$\frac{1}{N} \log \left[ \text{Tr} \ e^{-\beta H(J,h)} \right], \quad (1.5)$$

by use of a function which is a solution of a nonlinear integral equation. Thus, we can show that the expression of the free energy perfectly agrees with the results of TBA $[11]$.

The outline of this paper is the following. In §2, we derive an explicit expression of cluster expansion coefficients in all orders. In §3, we prove that the free energy can be expressed in terms of a solution of a nonlinear integral equation. The last section is devoted to the concluding remarks. Technical details of calculations are summarized in Appendices A-H.

### 2 The cluster expansion

The string hypothesis is formulated as follows. In the thermodynamic limit, the energy of the Heisenberg model (1.1) can be written as

$$E(J,h) = 2hM + \sum_{n,\alpha} \frac{2Jn}{(x_n^\alpha)^2 + n^2}. \quad (2.1)$$

Here, the variables $x_n^\alpha$ are determined by

$$\left( \frac{x_n^\alpha + ni}{x_n^\alpha - ni} \right)^N = \prod_{(m,\beta) \neq (n,\alpha)} E_{nm} (x_n^\alpha - x_m^\beta), \quad (2.2)$$

where

$$E_{nm}(x) = \frac{(x - (n + m)i)(x - |n - m|i)}{(x + (n + m)i)(x + |n - m|i)} \prod_{i=0}^{\min(n,m)} \left( \frac{x + (n + m - 2i)i}{x - (n + m - 2i)i} \right)^2. \quad (2.3)$$

Equation (2.2) is referred to as string center equation. Every eigenstate corresponds to a solution of these simultaneous equations. Taking a logarithm of both sides of (2.2), we
obtain
\[ 2N \tan^{-1} \left( \frac{x_n^\alpha}{n} \right) = 2\pi I_n^\alpha + \sum_{(m, \beta) \neq (n, \alpha)} \Delta_{n,m} (x_n^\alpha - x_m^\beta), \quad (2.4) \]
where
\[ \Delta_{n,m}(x) = -2\tan^{-1}\left( \frac{x}{n + m} \right) - 2(1 + \delta_{nm}) \tan^{-1}\left( \frac{x}{|n - m|} \right) + \sum_{l=0}^{\min(n,m)} 4\tan^{-1}\left( \frac{x}{n + m - 2l} \right). \quad (2.5) \]

From now on, we call \((2.4)\) modified Bethe Ansatz (mBA) equation.

The string hypothesis indicates that the partition function is a sum of the Boltzmann weights with respect to integers (or half integers) \(\{I_n^\alpha\}\) which define the energy of the system,
\[ z^{N/2} \text{Tr} e^{-\beta H(J,h)} = \sum_{\{I_n^\alpha\}} e^{-\beta E(J,h) - 2\beta h M}. \quad (2.6) \]

When we take the thermodynamic limit, we can replace the summations over discrete variables by integral,
\[ \int e^{-\beta E(J,h) - 2\beta h M} \prod dI_n^\alpha. \quad (2.7) \]

There are some points which we have to consider carefully. The Fermi statistics must be taken into account in this integral. In this case, the exclusion property leads to the conditions that \(x_n^\alpha \neq x_n^\beta\) and that a state specified by \(\{x_n^\alpha\}\) and a state specified by \(\{x_n^m\}\) which satisfies \(x_n^m = x_{p(\alpha)}^n\) are the same, where \(p\) is a permutation.

To express a concrete form of \((2.7)\), we prepare 3 symbols.

\begin{definition} 1. \end{definition}
\(N_A\) denotes the number of elements in a set \(A\).

\begin{definition} 2. \end{definition}
\(\Theta(A)\) denotes all the patterns of division of a set \(A\). A pattern of division is represented as a set having elements each of which is a cluster. The cluster is one of pieces into which a set \(A\) is divided, and the cluster is regarded as a set.

For example, for \(A = \{a, b, c\}\), \(\Theta(A)\) means
\[ \Theta(\{a, b, c\}) = \{\{a\}, \{b\}, \{c\}\}, \{\{a\}, \{b, c\}\}, \{\{b\}, \{c, a\}\}, \{\{c\}, \{a, b\}\}, \{\{a, b, c\}\}. \quad (2.8) \]
On condition that the domain of $\Theta(n)$ is the natural number, $n \in \mathbb{N}$, $\Theta(n)$ is interpreted as $\Theta(\{1, 2, \ldots, n\})$.

**Definition 3.**

$\bar{\Theta}(B)$ denotes all the patterns of division of a set $B$, when each element of $B$ is a set and each pattern of division satisfies the following condition; all the sets which are included in each cluster have the same number of elements. For example, we can show for $\sigma_1 = \{a, b\}, \sigma_2 = \{c\}, \sigma_3 = \{d\}$,

$$\bar{\Theta}(\{\sigma_1, \sigma_2, \sigma_3\}) = \{\{\sigma_1\}, \{\sigma_2\}, \{\sigma_3\}\}, \{\{\sigma_1\}, \{\sigma_2, \sigma_3\}\}. \quad (2.9)$$

Using the above symbols, the integral (2.7) can be written explicitly in the following form,

$$z^{N/2} \text{Tr} e^{-\beta H(J,h)} = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \bar{\Theta}(\theta)} \left[ \prod_{\theta' \in \zeta} (-1)^{N_{\theta'}-1} (N_{\theta'} - 1)! \right] \int \left| \frac{\partial I}{\partial x} \right|_{N,\zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'}. \quad (2.10)$$

We explain functions, $\left| \frac{\partial I}{\partial x} \right|_{N,\zeta}$ and $E(\zeta)$ used in this equation, where $\zeta \in \bar{\Theta}(\theta)$ and $\theta \in \Theta(n)$.

The Jacobian $\left| \frac{\partial I}{\partial x} \right|_{N,\zeta}$ is constructed as follows. First, we consider $\theta$ uniquely determined by the condition $\zeta \in \bar{\Theta}(\theta)$. Second, we make correspondence between each element $\sigma$ of $\theta$ and two suffixes $(n, \alpha)$ for the variables $I^n_\alpha$ and $x^n_\alpha$ introduced in the string hypothesis. In this case, the condition $N_{\sigma} = n$ is required. Third, we consider the mBA equation for the variables $\{I^n_\alpha\}, \{x^n_\alpha\}$ which are constructed out of $\theta$. Fourth, we introduce $x_{\theta'}, I_{\theta'}$, where $\theta'$ is an element of $\zeta$. Here, we have constraining conditions; $x_{\theta'} = x^n_\alpha$ and $I_{\theta'} = I^n_\alpha$, where $(n, \alpha)$ corresponds to $\sigma \in \theta'$. Finally, $\left| \frac{\partial I}{\partial x} \right|_{N,\zeta}$ is the Jacobian between $\{x_{\theta'}\}$ and $\{I_{\theta'}\}$ which satisfy respectively the mBA equation made from $\theta$ and the constraining conditions made from $\zeta$. Explicit expression of such Jacobian matrix is given in eq.(A.1). We show the above procedure by an example. For the case,

$$\zeta = \{\theta_1, \theta_2\}, \ \theta_1 = \{\{1, 2\}\}, \ \theta_2 = \{\{3\}, \{4\}\}, \quad (2.11)$$

we have

$$\theta = \{\{1, 2\}, \{3\}, \{4\}\}, \quad \zeta \in \bar{\Theta}(\theta)$$
\[ 2N \tan^{-1} \left( \frac{x_{\theta_1}}{2} \right) = 2\pi I_{\theta_1} + 2\Delta_{2,1} (x_{\theta_1} - x_{\theta_2}) \]
\[ 2N \tan^{-1} (x_{\theta_2}) = 2\pi I_{\theta_2} + \Delta_{1,2} (x_{\theta_2} - x_{\theta_1}) \]
\[ (2\pi)^2 \left| \frac{\partial I}{\partial x} \right|_{N,\zeta} = \frac{4N}{x_{\theta_1}^2 + 4x_{\theta_2}^2 + 1} \]
\[ \quad - \frac{4N}{x_{\theta_1}^2 + 4} \left( \frac{2}{(x_{\theta_1} - x_{\theta_2})^2 + 1} + \frac{6}{(x_{\theta_1} - x_{\theta_2})^2 + 9} \right) \]
\[ \quad - 2 \frac{2N}{x_{\theta_2}^2 + 1} \left( \frac{2}{(x_{\theta_2} - x_{\theta_1})^2 + 1} + \frac{6}{(x_{\theta_2} - x_{\theta_1})^2 + 9} \right). \] (2.12)

The energy \( E(\zeta) \) is expressed in terms of \( \{x^n_\alpha\} \) made from \( \theta \),
\[ E(\zeta) = \sum_{n,\alpha} \frac{2Jn}{(x^n_\alpha)^2 + n^2}, \] (2.13)
For the case (2.11), \( E(\zeta) \) is given by
\[ E(\zeta) = \frac{2J \times 2}{x_{\theta_1}^2 + 4} + \frac{2J}{x_{\theta_2}^2 + 1}. \] (2.14)

Note that the constraining conditions made from \( \zeta \) have been used.

Now, we show how (2.10) is derived. We notice two important facts. One is that, we must exclude unphysical states from the sum, when the sum is represented as the integral in (2.7). The unphysical state means the state corresponding to \( \{x^n_\alpha\} \) where some two elements of \( \{x^n_\alpha\} \) coincides, \( x^n_\alpha = x^n_\beta \). Those states should be excluded because the norm of the state constructed out of \( \{x^n_\alpha\} \) satisfying such a condition is zero. In eq.(2.10),
\[ \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \] (2.15)
are factors which exclude the unphysical states. In the expression (2.10), we add unphysical states in some terms of series and subtract them in some other terms. Then, the sum of positive terms and negative terms is zero with respect to unphysical states. This mathematical manipulation enables us to write the free energy explicitly like (2.10). Let us explain this manipulation for the case of \( \zeta \) in (2.11) in detail. The states corresponding to \( \zeta \) in (2.11) are unphysical states. We define \( \zeta' = \{\{1, 2\}\}, \{\{3\}\}, \{\{4\}\} \). \( \zeta' \) corresponds to the results of a string center equation (2.2) which defines one two-string \( x_{1,2} \) and two one-strings \( x_3, x_4 \). On the other hand, \( \zeta = \{\{1, 2\}\}, \{\{3\}\}, \{\{4\}\} \) in (2.11) corresponds to the results of the string center equation which satisfy \( x_3 = x_4 \). Therefore, the results corresponding to \( \zeta \) are part
of the results corresponding to \( \zeta' \). Here, in the sum with respect to elements in \( \bar{\Theta} \) (2.10), both \( \zeta \) and \( \zeta' \) are summed up. And, the sum of coordinates (2.13) of terms corresponding to both \( \zeta \) and \( \zeta' \) is zero. Therefore, unphysical states corresponding to \( \zeta \) do not affect the sum in (2.10). The other important fact is that, we must divide the sum by the number of the symmetry. Here, the symmetry means that when \( \{x^n_\alpha\} \) is a solution of the mBA equation, \( \{x'^n_\alpha\} \) which satisfies the relation \( x'^n_\alpha = x^n_{p(\alpha)} \) is also a solution of the mBA equation. In this case, it is necessary to divide the sum by the number of the symmetry because \( \{x^n_\alpha\} \) and \( \{x'^n_\alpha\} \) correspond to the same state. In eq.(2.10),

\[
\left[ \prod_{\sigma \in \theta} N\sigma! \right] / n! \tag{2.16}
\]

is a factor for the correction of the sum which takes such symmetry into account.

We have met similar correction factors in the analysis of the \( \delta \)-function bose gas system. The reason for the appearance of the correction factors is common. A detailed proof for the \( \delta \)-function bose gas system case is given in §3.1 [15].

In order to express the Jacobian \( \left| \frac{\partial l}{\partial x} \right|_{N,\zeta} \) explicitly, we further define three symbols.

\textit{definition 4.}

\( M_B \) denotes a number of elements in one of the sets. Here, all the elements of a set \( B \) are sets, and all sets in \( B \) have the same number of elements. Then, \( M_B \) is defined as the number of elements in one of the sets,

\[
M_\theta = N\sigma, \tag{2.17}
\]

where \( \sigma \in \theta \in \zeta \in \bar{\Theta} (\theta') \) and \( \theta' \in \Theta (n) \).

\textit{definition 5.}

\( \Lambda (A) \) denotes all the patterns of connection of a set \( A \). Here, what we call a pattern of connection satisfies the following two conditions. 1) Any two elements of \( A \) are connected or not. In other words, there is no multiple connection. 2) There is no closed path in the connections. Then, a pattern of connection is represented as a set of elements each of which corresponds to a connection. Here,
an element corresponding to a connection is a set which consists of two elements connected by the connection. For example, we have

\[
\Lambda (\{a, b, c\}) = \emptyset, \{\{b, c\}\}, \{\{c, a\}\}, \{\{a, b\}\}, \{\{a, b\}, \{a, c\}\}, \{\{b, a\}, \{b, c\}\}, \{\{c, a\}, \{c, b\}\}.
\]  

(2.18)

definition 6.

\(G(\[\lambda, A]\))\) is an element of \(\Theta(A)\), where \(\lambda \in \Lambda(A)\). In other words, \(G(\[\lambda, A]\))\) is a pattern of division of \(A\). The pattern of division \(\theta\) satisfies the following conditions; 1) any two connected elements are in the same set in \(\theta\), and 2) elements of \(\theta\) are larger in number than elements of any other \(\theta' \in \Theta(A)\) satisfying 1). For example, we can show that

\[
G (\{\{a, b\}, \{a, b, c\}\}) = \{\{a, b\}, \{c\}\}.
\]  

(2.19)

By use of the above three symbols, the Jacobian can be expressed as

\[
(2\pi)^{N_\zeta} \left| \frac{\partial I}{\partial x} \right|_{cN, \zeta} = \left[ \prod_{\theta \in \zeta} N_{\theta} \right]^{-1} \sum_{\lambda \in N(\zeta)} \left[ \prod_{\{\theta, \theta'\} \in \lambda} -N_{\theta}N_{\theta'}K_{M_{\theta}, M_{\theta'}} (x_\theta - x_{\theta'}) \right] \times \prod_{\zeta' \in G(\[\lambda, \zeta]\)} \left[ \sum_{\theta' \in \zeta'} \frac{2N_{\theta}M_{\theta}N}{M^2_{\theta} + x^2_{\theta'}} \right],
\]  

(2.20)

where \(K_{n,m}(x) \equiv d\Delta_{n,m}(x)/dx\). A proof of eq.(2.20) is given in Appendix A.

At last, we show the explicit expression of the cluster expansion. Taking a logarithm of both sides of (2.10) and rewriting the r.h.s., we get

\[
\log [z^{N/2} \text{Tr} e^{-\beta H(J,h)}] = \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_{\sigma} \right] \sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] \int \left| \frac{\partial I}{\partial x} \right|_{cN, \zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'}.
\]  

(2.21)

A proof is given in Appendix B. Here, \(\left| \frac{\partial I}{\partial x} \right|_{cN, \zeta}\) is the first order term of \(\left| \frac{\partial I}{\partial x} \right|_{N, \zeta}\) regarded as a polynomial with respect to the number of spins, \(N\). From the expression (2.21), the cluster expansion coefficient \(b_n\) is given by

\[
b_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_{\sigma} \right] \sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right].
\]
\[
\int \left| \frac{\partial I}{\partial x} \right|_{\infty, \zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'},
\]

where the explicit form of \( \left| \frac{\partial I}{\partial x} \right|_{cN, \zeta} \) is

\[
(2\pi)^N cN, \zeta \frac{\partial I}{\partial x} = \left[ \prod_{\theta \in \zeta} N_\theta \right]^{-1} \sum_{\lambda \in \Lambda_c(\zeta)} \left[ \prod_{\{\theta, \theta'\} \in \lambda} -N_\theta N_{\theta'} K_{M_\theta, M_{\theta'}} (x_\theta - x_{\theta'}) \right] \sum_{\theta \in \zeta} \frac{2N_\theta M_\theta N}{M_\theta^2 + x_{\theta}^2}.
\]

The symbol \( \Lambda_c(A) \) is defined as follows.

**definition 7.**

\( \Lambda_c(A) \) is a subset of \( \Lambda(A) \), where any element \( \lambda \in \Lambda_c(A) \) satisfies the condition \( N_G[\lambda, A] = 1 \). For example, we can show that

\[
\Lambda_c(\{a, b, c\}) = \{\{a, b\}, \{a, c\}, \{b, a\}, \{b, c\}, \{c, a\}, \{c, b\}\}.
\]

A derivation of the expression \( \left| \frac{\partial I}{\partial x} \right|_{cN, \zeta} \) in (2.23) is given in Appendix C.

### 3 The free energy

From eqs. (2.10) and (2.21), we can easily show that

\[
z^{1/2} \left[ \text{Tr} \ e^{-\beta H(J,h)} \right]^{1/N} = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] \int \left| \frac{\partial I}{\partial x} \right|_{1, \zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'},
\]

where \( \left| \frac{\partial I}{\partial x} \right|_{1, \zeta} \) means \( \left| \frac{\partial I}{\partial x} \right|_{cN, \zeta} \) in which \( N \) is replaced with 1.

Now, we introduce a function \( u(x) \),

\[
u(x) \equiv 1 + \sum_{n=1}^{\infty} z^n u_n(x),
\]

where \( u_n(x) \) is given by

\[
u_n(x) \equiv \frac{1}{n!} \sum_{\theta' \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] \int \left| \frac{\partial I}{\partial x} \right|_{1, \zeta} (x) e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'}
\]

(3.3)
with the modified Jacobian \( \left| \frac{\partial I}{\partial x} \right|_{1,\zeta}(y) \) defined as

\[
(2\pi)^N \left| \frac{\partial I}{\partial x} \right|_{1,\zeta}(y) \equiv \left[ \prod_{\theta \in \zeta} N_\theta \right]^{-1} \sum_{\lambda \in \Lambda(\zeta)} \left[ \prod_{(\theta,\theta') \in \lambda} -N_\theta N_{\theta'} K_{M_\theta,M_{\theta'}} (x_\theta - x_{\theta'}) \right] \prod_{\zeta' \in G(\lambda,\zeta)} \left[ \sum_{\theta \in \zeta'} \frac{2N_\theta M_\theta}{M_\theta^2 + (x_\theta - y)^2} \right].
\]

(3.4)

Comparing this definition with (2.20), it is readily seen that \( \left| \frac{\partial I}{\partial x} \right|_{1,\zeta} = \left| \frac{\partial I}{\partial x} \right|_{1,\zeta}(0) \). Then, it is clear that we can get a relation

\[
[\text{Tr} e^{-\beta H(J,h)}]^{1/N} = u(z^{-1/2}).
\]

(3.5)

It can be shown (see Appendix D for a proof) that the function \( u_n(x) \) satisfies the following recursion relation,

\[
u_{n+1}(x) = \oint_{0^+} \left[ \frac{\exp \left( -\frac{2J\beta}{(y+i)^2+1} \right)}{x - y - 2i} + \frac{\exp \left( -\frac{2J\beta}{(y-i)^2+1} \right)}{x - y + 2i} \right] \sum_{\theta \in \Theta(n)} \frac{N_\theta!}{n!} \left[ \prod_{\sigma \in \theta} -N_\sigma! u_{N_\sigma}(y) \right] \frac{dy}{2\pi i},
\]

(3.6)

\[
u_1(x) = 1 + \oint_{0^+} \left[ \frac{\exp \left( -\frac{2J\beta}{(y+i)^2+1} \right)}{x - y - 2i} + \frac{\exp \left( -\frac{2J\beta}{(y-i)^2+1} \right)}{x - y + 2i} \right] \frac{dy}{2\pi i},
\]

(3.7)

where \( n \) is the natural number. Using this recursion relation we obtain a relation

\[
u(x) = z + 1 + \oint_{0^+} \left[ \frac{\exp \left( -\frac{2J\beta}{(y+i)^2+1} \right)}{x - y - 2i} + \frac{\exp \left( -\frac{2J\beta}{(y-i)^2+1} \right)}{x - y + 2i} \right] \frac{z \ dy}{u(y) 2\pi i}.
\]

(3.8)

These results, (3.5) and (3.8), are the same as those of [11] in the XXX Heisenberg model limit.

### 4 Conclusion

We have shown a method, which we call direct method, to derive the free energy of the XXX Heisenberg model using the BA equation. The cluster expansion coefficient in arbitrary order is given for the first time. The expression of the free energy perfectly agrees with that by
TBA. It is remarkable that the free energy is obtained without recourse to TBA and QTM. On the other hand, there remains a problem. We have started from the string hypothesis in this paper. Therefore, it is still a challenging problem to derive each cluster expansion coefficient only from the BA equation. This problem is under investigation.

We think, however, that these results have theoretical significances. What we have done in this paper is that we calculate a certain summation using combinatorial argument with mathematical justification. The summation may contain a problem which comes from the string hypothesis. On the contrary, TBA solve this problem as follows. We define a non-equilibrium entropy, and minimize the free energy using such entropy. Then, the condition of minimization gives the summation. In other words, TBA entirely relies on the physical definition of the entropy. In this paper, it is proved that the two results by TBA and by the direct method are the same. Therefore, in addition to the δ-function bose gas, for the XXX Heisenberg model, the direct method gives the mathematical justification of TBA. To summarize, it is suggested that TBA can be systematically proved for many other integrable systems using combinatorial argument presented here.

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[17] M. Wadati and G. Kato, J. Phys. Soc. Jpn. 70 (2001) 1924.
Appendix A  Explicit form of Jacobian $\left| \frac{\partial I}{\partial x} \right|_{N,\zeta}$

In this appendix, we prove (2.20). Recall that $\left| \frac{\partial I}{\partial x} \right|_{N,\zeta}$ is the Jacobian defined for $\zeta \in \bar{\Theta}(\theta)$, where $\theta \in \Theta(n)$. The Jacobian matrix can be rewritten as follows; the Jacobian matrix has the order $N_{\zeta} \times N_{\zeta}$, and each element of the matrix is

$$\frac{2\pi}{M_{\theta}N_{\theta}} \left( \frac{N_{\theta}M_{\theta}}{M_{\theta}N_{\theta}} + \sum_{\theta' \neq \theta} N_{\theta'} K_{M_{\theta},M_{\theta'}}(x_{\theta} - x_{\theta'}) \right) \quad \text{if } \theta = \theta' \quad (A.1)$$

$$\frac{N_{\theta}M_{\theta}}{M_{\theta}N_{\theta}}(x_{\theta} - x_{\theta'}) \quad \text{if } \theta \neq \theta' , \quad$$

where $\theta, \theta', \theta'' \in \zeta$ and $K_{n,m}(x) \equiv d\Delta_{n,m}(x)/dx$.

Here, we generalize the setting of the problem. We define $N \times N$ matrix

$$A_{n,m} = \left\{ \begin{array}{ll} e_n - \sum_{k \neq n} c_k a_{n,k} & \text{if } n = m \\ c_n a_{n,m} & \text{if } n \neq m, \end{array} \right. \quad (A.2)$$

where $\{a_{n,m}\}, \{c_n\}$ and $\{e_n\}$ are arbitrary series and $a_{n,m}$ is symmetric, $a_{n,m} = a_{m,n}$. This matrix is a generalized form of the Jacobian matrix (A.1). Therefore, what we have to prove becomes that the determinant of $A_{n,m}$ is

$$|A_{n,m}| = \left[ \prod_{n=1}^{N} c_n \right]^{-1} \sum_{\lambda \in \Lambda([1,\ldots,N])} \left[ \prod_{(n,m) \in \lambda} -c_n c_m a_{n,m} \right] \prod_{\sigma \in G([\lambda,\{1,\ldots,N\}])} \left[ \sum_{n \in \sigma} c_n e_n \right]. \quad (A.3)$$

First, we prove that each term of the determinant $|A_{n,m}|$ can be considered as a pattern of connection $\lambda \in \Lambda([1,\ldots,N])$. When we regard the determinant as a multi-variable polynomial with respect to $\{a_{n,m}\}$ and regard $a_{n,m}$ as a connection between $n$ and $m$, we can consider each term of the polynomial as a pattern of connection $\lambda$. In other words, we can prove the following two facts. First, there is no multiple connection. That is to say, there is no $a_{n,m}$ to the power of 2 or more in any term of the polynomial. Second, there is no closed path made from connections. That is to say, there is no product $a_{p(1),p(2)} a_{p(2),p(3)} \cdots a_{p(M-1),p(M)} a_{p(M),p(1)}$ in any term, where $p$ is a permutation.

To prove these two facts, we use the method of false position. We assume there is a term that has at least one closed path through $M$ connections. Without loss of generality, the above assumption can be rewritten that there is a product $a_{1,2} a_{2,3} \cdots a_{M-1,M} a_{M,1}$ in any
term. Then, we introduce a matrix $A'_{n,m}$ such that

$$A'_{n,m} = \begin{cases} 
-\sum_{k \neq n} c_k a_{n,k} & \text{if } n = m \leq M \\
 e_n - \sum_{k \neq n} c_k a_{n,k} & \text{if } n = m > M \\
 0 & \text{if } n \leq M < m \text{ or } m \leq M < n \\
 c_n a_{n,m} & \text{other.} 
\end{cases} \quad \text{(A.4)}$$

Now, we regard $|A'_{n,m}|$ as a multi-variable polynomial with respect to $\{a_{n,m}\}$. From the definition of determinant, it is easily shown that the term with a product $a_{1,2}a_{2,3} \cdots a_{M-1,M}a_{M,1}$ in $|A_{n,m}|$ has the same coefficient as a term with such product in $|A'_{n,m}|$. However, $|A'_{n,m}|$ is identically 0 because the matrix $A'_{n,m}$ is linearly dependent. Therefore, there is no term containing a product $a_{1,2}a_{2,3} \cdots a_{M-1,M}a_{M,1}$. Substituting 2 for $M$, we can prove that there is no $a_{n,m}$ to the power of 2 or more in any term of the polynomial. Then, we can consider each term of the matrix $|A_{n,m}|$ as a pattern of connection $\lambda$.

Second, we find where a term considered as a pattern of connection is formed. From the definition, we can write the determinant $|A_{n,m}|$ as

$$|A_{n,m}| = \sum_{p \in P_N} \text{sgn} p \cdot \prod_{n=1}^{N} A_{n,p(n)}, \quad \text{(A.5)}$$

where $P_N$ is a permutation group with respect to $\{1, \cdots, N\}$. It can be shown that any term considered as a pattern of connection is in an expansion of a product only in the case $p$ is the identity permutation. The following is a proof of the fact by the method of false position. If there is such term in the case $p$ is not the identity permutation, there exist $n_0$ and $l_0$ which satisfy $p^{l_0}(n_0) = n_0$, $p^l(n_0) \neq n_0$ and $l_0 \neq 0$, where $l_0 > l$ and $p^m(n)$ means that $p$ operates on $n$ for $m$ times, $p(p(\cdots p(n) \cdots))$. Therefore, we can rewrite $\prod_{n=1}^{N} A_{n,p(n)}$ as

$$\left[ \prod_{l=0}^{l_0-1} c_{p^l(n_0)} a_{p^l(n_0),p^{l+1}(n_0)} \right] \prod_{n \neq p^l(n_0)} A_{n,p(n)}. \quad \text{(A.6)}$$

This term clearly has a closed path, and conflict with the definition of the $p$.

Finally, we can rewrite $|A_{n,m}|$ as follows. We expand

$$\prod_{n=1}^{N} A_{n,n}, \quad \text{(A.7)}$$
and regard it as a multi-variable polynomial with respect to \( \{a_{n,m}\} \). \( |A_{n,m}| \) is a sum of terms which are in this polynomial and can be considered as a pattern of connection. This means that the term has no multiple connection and no closed path. This sum means the r.h.s. of (A.3).

**Appendix B  
A proof of (2.21)**

In this appendix, we prove (2.21) from (2.10).

We define \( Z_n \) by

\[
z^{N/2} \text{Tr} \ e^{-\beta H(J,h)} \equiv 1 + \sum_{n=1}^{\infty} Z_n z^n. \tag{B.1}
\]

From (2.10) we get

\[
Z_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_\sigma! \sum_{\zeta \in \Theta(\theta)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] \int \left| \frac{\partial I}{\partial x} \right|_{N,\zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'}, \tag{B.2}
\]

where \( \left| \frac{\partial I}{\partial x} \right|_{N,\zeta} \) is the Jacobian defined for \( \zeta \). It is convenient to introduce \( f(\zeta) \) as

\[
f(\zeta) \equiv \int \left| \frac{\partial I}{\partial x} \right|_{N,\zeta} e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'}. \tag{B.3}
\]

Using this function and the relation (C.1) proved in Appendix C, we can rewrite \( Z_n \) as

\[
Z_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_\sigma! \sum_{\zeta \in \Theta(\theta)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} (N_{\theta'} - 1)! \right] \sum_{\xi \in \Theta(\zeta)} \prod_{\zeta' \in \xi} f(\zeta'). \tag{B.4}
\]

We also define \( b_n \) by

\[
\log \left[ 1 + \sum_{n=1}^{\infty} Z_n z^n \right] \equiv \sum_{n=1}^{\infty} b_n z^n. \tag{B.5}
\]

We can easily show the following relation between \( b_n \) and \( Z_n \),

\[
b_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} (N_{\theta} - 1)! (-1)^{N_{\theta} - 1} \prod_{\sigma \in \theta} N_\sigma! Z_{N_\sigma}. \tag{B.6}
\]

Substituting (B.4) for \( Z_n \) in (B.6), we get

\[
b_n = \frac{1}{n!} \sum_{\theta \in \Theta(n)} (N_{\theta} - 1)! (-1)^{N_{\theta} - 1}
\]
In the first equality, we have only performed the substitution. In the second equality, we have done the following manipulation. We regard each side of the equality as the sum with respect to elements in a set which satisfies some conditions. Therefore, we may change the order of the sums. Here, we show a simple example of “change of order”,

\[
\sum_{n=1}^{N} \sum_{m=1}^{n} f(\{n, m\}) = \sum_{m=1}^{N} \sum_{n=m}^{N} f(\{n, m\}).
\]  

(B.8)

Similar to this example, both sides of the second equality are the sum of the same function with respect to elements in the same set. In the third equality, we have simplified the last term of the l.h.s. using a relation,

\[
\sum_{\theta \in \Theta(\sigma)} (N_{\theta} - 1)!(-1)^{N_{\theta} - 1} = \delta_{N_{\theta}, 1}.
\]  

(B.9)

Finally, combining (B.1), (B.3), (B.5) and (B.7) we arrive at the equation (2.21).

Appendix C The structure of the Jacobian  

In this appendix, we prove

\[
\frac{\partial I}{\partial x}_{N, \zeta} = \sum_{\eta \in \Theta(\zeta)} \prod_{\zeta \in \zeta} \frac{\partial I}{\partial x}_{cN, \zeta}
\]  

(C.1)

and eq.(2.23) from eq.(2.20). We here repeat that  \(\frac{\partial I}{\partial x}_{cN, \zeta}\) is the first order term of  \(\frac{\partial I}{\partial x}_{N, \zeta}\) with respect to  \(N\).

Eq.(2.20) can be rewritten as

\[
(2\pi)^{N_\zeta} \frac{\partial I}{\partial x}_{N, \zeta} = \sum_{\eta \in \Theta(\zeta)} \prod_{\zeta' \in \zeta} N_\eta^{-1} \sum_{\lambda \in \Lambda(\zeta')} \prod_{\{\theta, \theta'\} \in \lambda} -N_\theta N_{\theta'} K_{M_\theta, M_{\theta'}} (x_\theta - x_{\theta'})
\]  

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\[
\sum_{\theta \in \zeta} \frac{2N_{\theta}M_{\theta}}{M_{\theta}^2 + x_{\theta}^2}.
\]  
\hspace{1cm} (C.2)

In this equality, we have changed the order of the sums. We can easily show the relation (2.28) from this expression. Then, eq.(C.2) and eq.(2.28) prove (C.1).

**Appendix D  A proof of (3.6) and (3.7)**

In this appendix, using the mathematical induction we prove the relations with respect to \(u_n(x)\), (3.6) and (3.7). The definition of \(u_n(x)\) is given in eq.(3.3).

We can change the r.h.s of (3.7) into
\[
\int_0^\infty \left[ \sum_{s=\pm 1} \prod_{\sigma \in \theta} -N_{\sigma}!u_{N_{\sigma}}(y - si) \right] e^{-\frac{2J\beta}{y^2+1}} \frac{dy}{2\pi i}.
\]  
\hspace{1cm} (D.1)

This is the same as the definition of \(u_1(x)\). Thus, we have shown the relation (3.7).

We suppose (3.6) and (3.7) hold for \(1 \leq n < n_0\), where \(n_0\) is a natural number. For simplicity, \(n_0\) is merely written as \(n\) in what follows. Then, the function \(u_m(x)\) has poles only at \(x = \pm 2i\), and satisfies \(\lim_{|x| \to \infty} u_m(x) = \delta_{m,1}\), where \(1 \leq m \leq n\). By use of these two properties, the r.h.s. of (3.6) becomes
\[
\int_{C_+} \left[ \prod_{\sigma \in \theta} -N_{\sigma}!u_{N_{\sigma}}(y - si) \right] e^{-\frac{2J\beta}{y^2+1}} \frac{dy}{2\pi i}.
\]
\hspace{1cm} (D.2)

In this equality we have changed the path of integration. Both \(C_+\) and \(C_-\) are the paths of integration which counterclockwise surround the region \(\Im y > 0\). When these paths are in the neighborhood of real axis, \(C_+\) passes above the real axis and \(C_-\) passes below the real axis. We separate (D.2) into two parts, and calculate them separately.

First, we consider the first term of (D.2) which is rewritten as
\[
\sum_{\theta \in \Theta(n)} \frac{N_{\theta}!}{n!} \int_{C_+} \left[ \prod_{\sigma \in \theta} -N_{\sigma}!u_{N_{\sigma}}(y - si) \right] e^{-\frac{2J\beta}{y^2+1}} \frac{dy}{2\pi i}.
\]
\hspace{1cm} (D.3)
The integral diverges in case that we do not sum up with respect to \( s \). However, the sum turns out not to play an important role in the following calculation. Hence, to shorten the expression, a symbol \( \sum_{s=\pm} \) is omitted for a while. Now, by use of the relation (E.1) proved in Appendix E, eq.(D.3) is rewritten as

\[
\frac{1}{n!} \int_{-\infty + s\delta i}^{\infty + s\delta i} \frac{dy}{2\pi} \sum_{\theta \in \Theta(n)} \prod_{\sigma \in \theta} \left[ - \sum_{\theta' \in \Theta(\sigma)} \prod_{\sigma' \in \theta'} N_{\sigma'}! \right] \sum_{\zeta \in \Theta(\theta')} (\prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1}) \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \\
\prod_{\theta' \in \zeta} \int_{-\infty}^{\infty} \frac{dx_{\theta'}}{2\pi} \sum_{\lambda \in \Lambda(\zeta)} \prod_{\{\theta', \theta''\} \in \lambda} -N_{\theta''} N_{\theta'''} K_{M_{\theta''}, M_{\theta'''}} (x_{\theta''} - x_{\theta'''}) \\
\sum_{\theta'' \in \zeta} 2N_{\theta''} M_{\theta''} + (x_{\theta''} - y + si)^2 s - (y - x)i \right].
\]

(D.4)

On condition that we take a limit \( \delta \to 0 \) and \( M_\theta = 1, 1/(M_\theta^2 + (x_\theta - y + si)^2) \) yields a pole on the real axis with respect to the variable \( y \). To detour the pole on the real axis and symmetrize the integral paths, we use the relation (E.1) proved in Appendix E. Then, (D.4) becomes

\[
\frac{1}{n!} \sum_{\theta \in \Theta(n)} \prod_{\sigma \in \theta} N_{\sigma}! \sum_{\zeta \in \Theta(n+1)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'} - 1} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \frac{N_{\theta_{n+1}}}{(N_{\theta_{n+1}} - 1)!} \\
\prod_{\zeta' \in \Theta(n+1)} B_{N_{\zeta'}} \prod_{\theta' \in \zeta'} (N_{\theta'} - 1)! \int_{\text{sym}} \prod_{\theta' \in \zeta'} \frac{dx_{\theta'}}{2\pi} \sum_{\lambda \in \Lambda(\zeta)} \frac{s e^{-\beta E(\zeta)}}{s - (x_{\theta_{n+1}} - x) i} \\
\prod_{\{\theta', \theta''\} \in \lambda} C(\theta', \theta'') \prod_{\{\theta_{n+1}, \theta'\} \in \lambda} E(\theta_{n+1}, \theta') .
\]

(D.5)

Here, we assume the relation \( \{n+1\} \in \sigma_{n+1} \in \theta_{n+1} \in \zeta \). We also use this symbol in the same sense as in (D.12), (D.19) and (D.20). The constant \( B_n \) in (D.3) is known as the Bernoulli number and is determined by

\[
\sum_{n=0}^{\infty} \frac{B_n}{n!} x^n \equiv \frac{x}{1 - e^{-x}}.
\]

(D.6)

For example, first few \( B_n \)'s are

\[
B_0 = 1 \quad , \quad B_1 = \frac{1}{2} \quad , \quad B_2 = \frac{1}{6} \quad , \quad B_3 = 0 \quad , \quad B_4 = -\frac{1}{30} \quad , \quad \ldots.
\]

(D.7)
The symbol $\int_{\text{sym}}$ in \((\text{D.3})\) indicates that each path of integration symmetrically avoids poles on the real axis. Because all the poles on the real axis have the form $1/(x_\theta - x_{\theta'})$, we can write explicitly $\int_{\text{sym}}$ as

$$
\int_{\text{sym}} \prod_{n=1}^{N} dx_n \equiv \frac{1}{N!} \sum_{\{p \in P_n\}} \prod_{n=1}^{N} \left[ \int_{-\infty+\text{i}n\delta}^{\infty+\text{i}n\delta} dx_{\rho(n)} \right].
$$

(D.8)

The functions $C(\theta, \theta')$ and $E(\theta, \theta')$ are defined by

$$
C(\theta, \theta') \equiv -N_\theta, N_\theta' K_{M_\theta, M_\theta'} (x_\theta - x_{\theta'}),
$$

(D.9)

$$
E(\theta, \theta') \equiv -(N_\theta - 1) N_\theta' K_{M_\theta, M_\theta'} (x_\theta - x_{\theta'}) - N_\theta' K_{M_\theta - 1, M_\theta'} (x_\theta - x_{\theta'} - si)
- \frac{2N_\theta M_{\theta'}}{M_{\theta'}^2 + (x_\theta - x_{\theta'} + s(\theta_{\theta'} - 2)i)^2}.
$$

(D.10)

Note here that the second term of \((\text{D.10})\) is 0 for $E(\theta, \theta')$ used in \((\text{D.3})\) because of the relation $M_{\theta_{n+1}} = 1$. Then, by use of the relation

$$
\sum_{\theta \in \Theta(n)} B_{N_\theta} \prod_{\sigma \in \theta} (N_\sigma - 1)! = \frac{n!}{n + 1},
$$

(D.11)

which is easily shown, \((\text{D.3})\) becomes

$$
\frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\xi \in \Theta(\theta \cup \{n+1\})} \left[ \prod_{\theta' \in \xi} (-1)^{N_{\theta'} - 1} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \right] \frac{1}{N_{\theta_{n+1}}} \int_{\text{sym}} \prod_{\theta' \in \xi} \frac{dx_{\theta'} \theta}{2\pi}
$$

$$
\sum_{\chi \in A(\xi)} \frac{sN_{\theta_{n+1}} e^{-\beta E(\xi)}}{s - (x_{\theta_{n+1}} - x)} i \left[ \prod_{\theta' \in \xi} C(\theta', \theta'') \right] \left[ \prod_{\{\theta_{n+1}, \theta'\} \in \lambda} E(\theta_{n+1}, \theta') \right].
$$

(D.12)

Changing the order of the sums, this expression becomes

$$
\frac{1}{(n + 1)!} \sum_{\theta \in \Theta(n+1)} \left[ \prod_{\sigma \in \theta} N_\sigma! \right] \sum_{\xi \in \Theta(\theta)} \left[ \prod_{\theta' \in \xi} (-1)^{N_{\theta'} - 1} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \right] \int_{\text{sym}} \prod_{\theta' \in \xi} \frac{dx_{\theta'} \theta}{2\pi}
$$

$$
\sum_{\chi \in A(\xi)} \sum_{\theta_0 \in \xi, M_{\theta_0} = 1} \frac{sN_{\theta_0} e^{-\beta E(\xi)}}{s - (x_{\theta_0} - x)} i \left[ \prod_{\theta', \theta'' \in \xi} C(\theta', \theta'') \right] \left[ \prod_{\{\theta_0, \theta'\} \in \lambda} E(\theta_0, \theta') \right].
$$

(D.13)

Thus, using the above relations we have shown that \((\text{D.3})\) is expressed as \((\text{D.13})\).

Second, we write the sum of the second and third terms of \((\text{D.2})\),

$$
- \sum_{s=\pm 1} s \sum_{\theta \in \Theta(n)} \frac{N_\theta!}{n!} \int_{C_s} \prod_{\sigma \in \theta} -N_\sigma! u_{N_\sigma} (y) e^{-\frac{2\pi j s}{(y + \text{i}n\delta)^2}} dy
- \frac{2\pi j s}{(y + \text{i}n\delta)^2}.
$$

(D.14)
where, $C_{\pm 1}$ means $C_{\pm}$. In the following change of the expressions, the sum with respect to $s$ does not play an important role. This situation is similar to the one for (D.3). Then, the symbol $\sum_{s=\pm 1}$ will be also omitted for a while. Using the relation (E.1), we have from (D.14),

$$-rac{1}{n!} \int_{C_s} \frac{dy}{2\pi} \sum_{\theta' \in \Theta (n)} \prod_{\sigma \in \theta} \left[ - \sum_{\theta'' \in \Theta (\sigma)} \left[ \prod_{\lambda' \in \theta''} \frac{N_{\lambda''}!}{N_{\lambda''}!' (N_{\lambda''} - 1)!} \sum_{\lambda'' \in \Theta (\lambda'')} \prod_{\theta'' \in \lambda''} (-1)^{N_{\theta''} - 1} \frac{(N_{\theta''} - 1)!}{N_{\theta''}} \right] \prod_{\lambda' \in \lambda''} \frac{2N_{\lambda'} M_{\lambda'}}{M_{\lambda'}^2 + (x_{\lambda'} - y)^2} s - \frac{\beta (2j)^2 + E(\zeta)}{2s - (y - x)i} \right].$$

We use a relation,

$$\int_{C_s} dy f (y) \prod_{\sigma \in \theta} \left[ \int_{-\infty}^{\infty} dx_{\sigma} \frac{2N_{\sigma} f_{\sigma} (x_{\sigma})}{2N_{\sigma}^2 + (y - x_{\sigma})^2} \right] = \int_{C_s} dy f (y + msi) \prod_{\sigma \in \theta} \left[ \int_{-\infty}^{\infty} dx_{\sigma} \frac{2N_{\sigma} f_{\sigma} (x_{\sigma})}{2N_{\sigma}^2 + (y - x_{\sigma} + msi)^2} \right] + \sum_{n=0}^{m-1} \int_{C_s} dy f (y + nsi) \prod_{\sigma \in \theta} \int_{-\infty}^{\infty} dx_{\sigma} \frac{2N_{\sigma} f_{\sigma} (x_{\sigma})}{2N_{\sigma}^2 + (y - x_{\sigma} + nsi)^2} - \prod_{\sigma \in \theta} \int_{-\infty}^{\infty} dx_{\sigma} \frac{2N_{\sigma} f_{\sigma} (x_{\sigma})}{2N_{\sigma}^2 + (y - x_{\sigma} + nsi)^2} - \delta (n + 1, N_{\sigma}) f_{\sigma} (y - si),$$

where $f_{\sigma}(x)$ and $f(x)$ are analytic functions in the regions $-1 < \Im x \leq 0$ and $0 < \Im x \leq m$ in case of $s = 1$ ($0 \leq \Im x < 1$ and $-m \leq \Im x < 0$ in case of $s = -1$) respectively, and $\max_{\sigma \in \theta} N_{\sigma} = m$. Then, (D.15) becomes

$$\frac{1}{n!} \sum_{\theta' \in \Theta (n)} \prod_{\sigma' \in \theta'} \frac{N_{\sigma'}!}{N_{\sigma'}!' (N_{\sigma'} - 1)!} \sum_{\theta'' \in \Theta (\theta')} \prod_{\lambda'' \in \lambda''} \frac{(-1)^{N_{\lambda''} - 1} (N_{\lambda''} - 1)!}{N_{\lambda''}!' (N_{\lambda''} - 1)!} \sum_{\theta'' \in \lambda''} N_{\theta''} (N_{\theta''} - 1)! \prod_{\lambda'' \in \lambda''} \frac{\int_{C_s} dx_{\lambda''}}{2\pi} \left[ \prod_{\theta'' \in \lambda''} \frac{2N_{\lambda''} M_{\lambda''}}{M_{\lambda''}^2 + (x_{\lambda''} - y)^2} \right] \prod_{\lambda'' \in \lambda''} \frac{2N_{\lambda''} M_{\lambda''}}{M_{\lambda''}^2 + (x_{\lambda''} - x_{\lambda''} + s (M_{\lambda''} - 1)i)^2} \prod_{\{\theta'', \theta''\}} C (\theta'', \theta'') \prod_{\{\lambda'' \}} \frac{E (\zeta) + \frac{2j}{(x_{\lambda''} + M_{\lambda''}) + 1} + \frac{2j M_{\lambda''}}{(x_{\lambda''} - s i)^2 + M_{\lambda''}^2} - \frac{2j M_{\lambda''}}{x_{\lambda''}^2 + M_{\lambda''}^2}}{(M_{\lambda''} + 1) s - (x_{\lambda''} - x)i}.$$
We point out that in this case the first term of the r.h.s. in (D.16) is 0 because there is no pole inside (outside) the path of integration \( C_+ (C_-) \) with respect to \( y \) including the point \(|y| = \infty\). Then, using a simple relation \( \sum_{\theta \in \Theta_n} \prod_{\sigma \in \theta} (-1)^{N_{\sigma}^{-1}} (N_{\sigma} - 1)! = \delta_{n,1} \), we get from (D.17),

\[
\frac{1}{n!} \sum_{\theta \in \Theta(n)} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\sigma \in \theta} \sum_{\zeta \in \Theta(\theta - \sigma)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'}^{-1}} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \int_{-\infty}^{+\infty} \frac{dx_{\theta}}{2\pi} \int_{-\infty}^{+\infty} \frac{dx_{\theta'}}{2\pi} \left[ \prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right] \sum_{\lambda \in \Lambda(\zeta + \theta_0)} \left[ \prod_{\theta', \theta''} \frac{s \exp \left[ -\beta \left( E(\zeta) + \frac{2J(M_{\theta_0}+1)}{x_{\theta_0}^2 + (M_{\theta_0}+1)^2} - \frac{2JM_{\theta_0}}{x_{\theta_0}^2 + M_{\theta_0}^2} \right) \right]}{(M_{\theta_0} + 1) s - (x_{\theta_0} - x) i} \right] C(\theta', \theta'') E(\theta_{n+1}, \theta) \right], \tag{D.18}
\]

where \( \theta_0 \equiv \{ \sigma_0 \} \). Here, we have changed the path of integration from \( C_s \) to \( -\infty + s\delta i \to +\infty + s\delta i \), because there is no pole at \(|x_{\theta_0}| \to \infty\). In eq.(D.18), when we take a limit \( \delta \to 0 \) and \( M_{\theta} = M_{\theta_0} + 1 \), the last term contains a pole on the real axis with respect to \( x_{\theta_0} \).

Symmetrizing by use of (F.11) the integral paths which avoid the pole on the real axis, we obtain from (D.18).

\[
\frac{1}{n!} \sum_{\theta \in \Theta(n+1), \sigma_{n+1} \neq 1} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'}^{-1}} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \frac{N_{\theta_{n+1}}}{N_{\sigma_{n+1}} (N_{\sigma_{n+1}} - 1)!} \left[ \sum_{\theta' \in \Theta(N_{\theta_{n+1}}-1)} \prod_{\sigma' \in \theta'} (N_{\sigma'} - 1)! \int_{\text{sym}} \prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right] \sum_{\lambda \in \Lambda(\zeta)} \frac{s \exp \left[ E(\zeta) \right]}{(M_{\theta_{n+1}} + 1) s - (x_{\theta_{n+1}} - x) i} \left[ \prod_{\theta_{n+1}, \theta'} C(\theta', \theta'') \right] \left[ \prod_{\{\theta_{n+1}, \theta'\} \in \lambda} E(\theta_{n+1}, \theta') \right], \tag{D.19}
\]

By use of (D.11), (D.19) is written as

\[
\frac{1}{n!} \sum_{\theta \in \Theta(n+1), \sigma_{n+1} \neq 1} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'}^{-1}} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \frac{1}{N_{\sigma_{n+1}} N_{\theta_{n+1}}} \int_{\text{sym}} \prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \left[ \prod_{\theta_{n+1}, \theta'} C(\theta', \theta'') \right] \left[ \prod_{\{\theta_{n+1}, \theta'\} \in \lambda} \frac{s \exp \left[ E(\zeta) \right]}{M_{\theta_{n+1}} s - (x_{\theta_{n+1}} - x) i} \left[ \prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right] \right], \tag{D.20}
\]

Changing the order of the summations, this expression becomes

\[
\frac{1}{(n+1)!} \sum_{\theta \in \Theta(n+1)} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \prod_{\theta' \in \zeta} (-1)^{N_{\theta'}^{-1}} \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \int_{\text{sym}} \prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \]
\[
\sum_{\lambda \in \Lambda_0} \sum_{\theta_0 \in \zeta, M_0 \neq 1} \frac{sN_{\theta_0} e^{E(\zeta)}}{M_{\theta_0} s - (x_{\theta_0} - x)^i} \left[ \prod_{\lambda, \theta, \theta' \neq \theta_0} C(\theta', \theta) \right] \left[ \prod_{\{\theta_0, \theta'\} \in \lambda} E(\theta_0, \theta') \right]. \tag{D.21}
\]

From the above relations we see that (D.12) is equal to (D.21).

Both parts of the r.h.s. of (D.2) are replaced with (D.12) and (D.21). Then, the r.h.s. of (D.2) is expressed as
\[
\frac{1}{(n + 1)!} \sum_{\theta \in \Theta(n + 1)} \left[ \prod_{\sigma \in \theta} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta' \in \zeta} (-1)^N_{\theta'} - 1 \frac{(N_{\theta'} - 1)!}{N_{\theta'}} \right] \int_{\text{sym}} \left[ \prod_{\theta' \in \zeta} \frac{dx_{\theta'}}{2\pi} \right] \sum_{\lambda \in \Lambda_0} \sum_{s = 1} \frac{sN_{\theta_0} e^{E(\zeta)}}{M_{\theta_0} s - (x_{\theta_0} - x)^i} \left[ \prod_{\lambda, \theta, \theta' \neq \theta_0} C(\theta', \theta) \right] \left[ \prod_{\{\theta_0, \theta'\} \in \lambda} E(\theta_0, \theta') \right]. \tag{D.22}
\]

Using eq. (G.1) proved in Appendix G, we can confirm the definition of \( u_{n+1}(x) \), which is the r.h.s. of (B.6).

**Appendix E**  
An expression of \( u_n(x) \)

In this appendix, we prove the following expression of \( u_n(x) \),
\[
\sum_{\theta \in \Theta(n)} \frac{N_{\theta}!}{n!} \prod_{\sigma \in \theta} N_{\sigma}! u_{N_{\sigma}}(y)
= \frac{1}{n!} \sum_{\theta \in \Theta(n)} \prod_{\sigma \in \theta} \left[ - \sum_{\theta' \in \Theta(\sigma)} \prod_{\theta'' \in \sigma \theta'} N_{\sigma}! \right] \sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta'' \in \zeta} (-1)^N_{\theta''} - 1 \frac{(N_{\theta''} - 1)!}{N_{\theta''}} \right] \int \left[ \frac{\partial I}{\partial x} \right]_{c_{1, \zeta}} (y) e^{-\beta E(\zeta)} \prod_{\theta' \in \zeta} dx_{\theta'} \right]. \tag{E.1}
\]

Here, the definition of \( u_n(x) \) is (B.3), and the definition of \( \left[ \frac{\partial I}{\partial x} \right]_{c_{1, \zeta}} \) is
\[
(2\pi)^N_{\zeta} \left. \frac{\partial I}{\partial x} \right|_{c_{1, \zeta}} (y)
= \left[ \prod_{\theta \in \zeta} N_{\theta} \right]^{-1} \sum_{\lambda \in \Lambda_0} \left[ \prod_{\theta, \theta' \in \lambda} -N_{\theta} N_{\theta'} K_{M_\theta, M_{\theta'}} (x_\theta - x_{\theta'}) \right] \sum_{\theta \in \zeta} \frac{2N_{\theta} M_{\theta}}{M_{\theta}^2 + (x_\theta - y)^2}. \tag{E.2}
\]

Substituting (B.3) for \( u_{N_{\sigma}}(y) \) in the l.h.s. of (E.1) and using a relation
\[
\left[ \frac{\partial I}{\partial x} \right]_{c_{1, \zeta}} (y) = \sum_{\xi \in \Theta(\zeta)} \prod_{\zeta' \in \xi} \left[ \frac{\partial I}{\partial x} \right]_{c_{1, \zeta'}} (y), \tag{E.3}
\]

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which is proved in the same way as (C.1), we can show that the l.h.s. of (E.1) is calculated as

\[
\sum_{\theta \in \Theta(n)} N_{\theta}! \prod_{\sigma \notin \theta} \left[ - \sum_{\theta' \in \Theta(\sigma)} \left( \prod_{\sigma' \in \theta'} N_{\theta'}! \right) \sum_{\zeta \in \Theta(\theta')} \left( \prod_{\sigma' \in \zeta} (N_{\theta'} - 1)! \right) \right] \sum_{\theta'' \in \zeta} \left[ \prod_{\sigma' \in \zeta} (N_{\theta''} - 1)! \right] \]

\[
\sum_{\zeta \in \Theta(\theta)} \left[ \prod_{\theta' \in \zeta} \left( - \sum_{\theta'' \in \Theta(\sigma)} \left[ \prod_{\sigma' \in \theta''} (N_{\theta''} - 1)! \right] \right) \prod_{\theta' \in \zeta} (N_{\theta'}! \right) \right] \int \frac{\partial I}{\partial x} e^{-\beta E(\zeta')} \prod_{\theta' \in \zeta} dx_{\theta'} \].

(E.4)

In this equality, we have changed the order of the sums. Using a relation

\[\sum_{\theta \in \Theta(n)} N_{\theta}!(-1)^{N_{\theta}} = (-1)^{n}\]  

for simplification of the first term of (E.4), we obtain the r.h.s. of (E.1).

**Appendix F  Symmetrization of the paths of integrals**

In this appendix, we prove a relation,

\[
\int_{-\infty}^{\infty} dx f_0(x) \prod_{n=1}^{N} \left[ \sum_{m=0}^{N_n} \left( \frac{1}{y_n - x} f_n(y_n) \right) \right] \]

\[
= \sum_{\sigma \subseteq \{1, \ldots, N\}} B_{\sigma} \int_{\text{sym}} f_0(x) \left[ \prod_{n \in \sigma} f_n(x) \right] \prod_{n \in \{1, \ldots, N\} - \sigma} \left( \frac{1}{y_n - x} f_n(y_n) \right) dx. \quad (F.1)
\]

Here, the definitions of \(B_{\sigma}\) and \(\int_{\text{sym}}\) are in (D.6) and (D.8) respectively, and we assume that \(f_n(x)\) is an analytic function on the real axis.

The paths of integrations in the r.h.s. of (F.1) are changed into ones in the l.h.s. of (F.1). In other words, symmetrical paths of integrations are changed into ones which keep the relation \(\Im y_n < \Im x\). Then, the r.h.s. of (F.1) becomes

\[
\sum_{\sigma \subseteq \{1, \ldots, N\}} \left[ \sum_{m=0}^{N_{\sigma}} \left( \frac{1}{(N_{\sigma} - m)!} \right) \prod_{l=0}^{N_{\sigma} - m} \left( \frac{(l + N_{\sigma} - m)!}{l!} (N - N_{\sigma})! \right) B_m \right]
\]
\[ \int_{-\infty+\delta i}^{\infty+\delta i} dx f_0(x) \left[ \prod_{n \in \sigma} f_n(x) \right] \prod_{n \in \{1, \ldots, N\} - \sigma} \left[ \int_{-\infty}^{\infty} \frac{dy_n}{2\pi i} \frac{1}{y_n - x} f_n(y_n) \right]. \] (F.2)

Using the following two relations which are easily shown,
\[
\sum_{l=0}^{n} \frac{(l+m)!}{l!} = \frac{(n+m+1)!}{n!(m+1)} \quad (F.3)
\]
\[
\sum_{m=0}^{n} (-1)^{n-m} \frac{n!}{(n-m+1)!m!} B_m = \delta_{n,0} \quad (F.4)
\]

for (F.2), we obtain the l.h.s. of (F.1).

**Appendix G  Alternative representation of the modified Jacobian**

In this appendix, we show that

\[
(2\pi)^{N_\zeta} \left| \frac{\partial I}{\partial x} \right|_{1,\zeta} (y) = \left[ \prod_{\theta \in \zeta} N_\theta \right]^{-1} \sum_{\lambda \in \Lambda_\zeta(\zeta)} \sum_{\theta \in \zeta} \sum_{s=1}^{\lambda} \frac{sN_\theta}{sM_\theta - (x_\theta - y)i} \left[ \prod_{\{\theta',\theta''\} \in \lambda} C(\theta',\theta'') \right] \left[ \prod_{\{\theta',\theta''\} \in \lambda} E(\theta,\theta') \right] \quad (G.1)
\]

is an alternative representation of the modified Jacobian (3.4). Here, \(C(\theta,\theta')\) and \(E(\theta,\theta')\) are defined in (D.9) and (D.10) respectively.

We can rewrite (3.4) as

\[
(2\pi)^{N_\zeta} \left| \frac{\partial I}{\partial x} \right|_{1,\zeta} (y) = \left[ \prod_{\theta \in \zeta} N_\theta \right]^{-1} \sum_{\lambda \in \Lambda_\zeta(\zeta)} \sum_{\theta \in \zeta} \sum_{s=1}^{\lambda} \frac{sN_\theta}{sM_\theta - (x_\theta - y)i} \left[ \prod_{\{\theta',\theta''\} \in \lambda} C(\theta',\theta'') \right] \left[ \prod_{\{\theta',\theta''\} \in \lambda} E(\theta,\theta') \right] \quad (G.2)
\]
In the first equality, we have changed the order of the sums. In the second equality, we have used the relation (H.1) proved in Appendix H. Applying a relation
\[ K_{M\theta, M\theta'}(x\theta - x\theta') - \frac{2M\theta'}{M_{\theta'}^2 + (x\theta' - x\theta - sM\theta i)^2} \]
\[ = K_{M\theta-1, M\theta'}(x\theta - x\theta' - si) + \frac{2M\theta'}{M_{\theta'}^2 + (x\theta - x\theta' + s(M\theta - 2)i)^2} \]
\[ (G.3) \]
to (G.2), we obtain the r.h.s. of (G.1). In the relation (G.3), it is supposed that \( s \) is \( \pm 1 \).

**Appendix H  A Proof of a fractional relation**

In this appendix, we prove
\[ \sum_{n=1}^{N} \sum_{\sigma \subseteq \{1, \ldots, N\} - \{n\}} \frac{1}{N - N_\sigma} \left[ \prod_{m \in \sigma} c_m \right] \left[ \prod_{m \subseteq \{1, \ldots, N\} - \sigma} \frac{2a_m d_m}{a_m^2 + (y - x_m)^2} \right] \]
\[ = \sum_{s=\pm 1} \sum_{n=1}^{N} s a_n - (x_n - y)i \prod_{m \neq n} \left[ c_m + \frac{2a_m d_m}{a_m^2 + (x_m - x_n - s a_n i)^2} \right], \]
\[ (H.1) \]
where \( a_n, c_n, d_n, x_n \) and \( y \) are arbitrary numbers.

We first prove a relation
\[ 1 = \sum_{n=1}^{N} \prod_{m \neq n} \frac{s_m a_m - (x_m - y)i}{s_m a_m - s_n a_n - (x_m - x_n)i}. \]
\[ (H.2) \]
We regard the r.h.s. as a polynomial of degree \( N - 1 \) with respect to \( y \). It is clear that this relation holds on the \( N \) points \( y = x_n + s_n a_n i \). Therefore, this equation is nothing but an identical equation. Dividing both sides of this identical equation by \( \prod_{n=1}^{N} [a_n - s_n (x_n - y) i] d_n^{-1} \), we get
\[ \prod_{n=1}^{N} \frac{s_n d_n}{s_n a_n - (x_n - y)i} = \sum_{n=1}^{N} \frac{s_n d_n}{s_n a_n - (x_n - y)i} \prod_{m \neq n} \frac{s_m d_m}{s_m a_m - s_n a_n - (x_m - x_n)i}. \]
\[ (H.3) \]
Here, we restrict that \( s_n \) is \( \pm 1 \). The sum of each side of this equation with respect to \( \{s_n\} \) gives
\[ \prod_{n=1}^{N} \frac{2a_n d_n}{a_n^2 + (y - x_n)^2} = \sum_{s=\pm 1} \sum_{n=1}^{N} s a_n - (x_n - y)i \prod_{m \neq n} \frac{2a_m d_m}{a_m^2 + (x_m - x_n - s a_n i)^2}. \]
\[ (H.4) \]
We are in a position to prove the main issue of this Appendix. Using (H.4) for the l.h.s. of (H.1), we get

\[
\sum_{s=\pm 1} \sum_{n=1}^{N} s \alpha_n \left[ \prod_{m \in \sigma} c_m \right] \left( \prod_{m \in \{1, \ldots, N\} - \{n\} - \sigma} a_m^2 + \left( x_m - x_n - sa_n i \right)^2 \right)
\] (H.5)

Expanding the r.h.s. of (H.1), we also get (H.5). This completes a proof of (H.1).