A note on the high temperature expansion of the density matrix for the isotropic Heisenberg chain

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Abstract

Göhmann, Klümper and Seel derived the multiple integral formula of the density matrix of the XXZ Heisenberg chain at finite temperatures. We have applied the high temperature expansion (HTE) method to isotropic case of their formula in a finite magnetic field and obtained coefficients for several short-range correlation functions. For example, we have succeeded to obtain the coefficients of the HTE of the 3rd neighbor correlation function \( < \sigma_j^z \sigma_{j+3}^z > \) for zero magnetic field up to the order of 25. These results expand our previous results on the emptiness formation probability [Z.Tsuboi, M.Shiroishi, J. Phys.A: Math. Gen. 38(2005) L363] to more general correlation functions.

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1 Introduction

Göhmann, Klümper and Seel derived [1] (see also [2, 3, 4, 5]) a multiple integral formula of matrix elements of a density matrix of a finite segment

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of arbitrary length $m$ of the anti-ferromagnetic spin $1/2$ $XXZ$ Heisenberg infinite chain at finite temperature in a finite magnetic field by combining the quantum transfer matrix approach \[6\]-\[10\] and the algebraic Bethe ansatz technique. Their formula generalizes the multiple integral formulae for zero temperature \[11\] \[12\] \[13\] to finite temperature case. This is a fundamental quantity since thermal average of any operators acting non-trivially on the segment of length $m$ can be expressed in terms of their formula. Thus it is an important problem to perform this multiple integral and extract concrete numbers from it. Their formula contains an auxiliary function, which is a solution of a nonlinear integral equation. This nonlinear integral equation is essentially same as the one for the free energy \[8\] \[9\]. Thus to evaluate their formula consists of two non-trivial tasks: to solve the nonlinear integral equation and to integrate the multiple integrals. In our previous paper \[14\], we applied the high temperature expansion (HTE) method to a multiple integral formula \[3\] of the emptiness formation probability $P(m)$ for the $XXX$ model, which is the probability of $m$ adjacent spins being aligned upward, and succeeded to obtain the coefficients of $P(3)$ up to the order of 42. As for zero magnetic field case, there is also numerical calculation \[15\] for the multiple integral for $m = 2, 3$. The purpose of this paper is to expand our previous results on the HTE for $P(m)$ \[14\] to more general correlation functions for the spin $1/2$ isotropic Heisenberg chain in a magnetic field $h$. In section 2, we introduce the multiple integral formula of the matrix elements of the density matrix \[11\]. In section 3, we evaluate this multiple integral by the HTE method. Based on the result of the HTE of the density matrix, we will calculate the HTE of two point correlation functions \(3.1)-(3.3)\). In particular for zero magnetic field case, we have succeeded to obtain the coefficients of the HTE of a 3rd neighbor correlation function up to the order of 25 (cf. eq. \(3.10)\)). Section 4 is devoted to concluding remarks.

## 2 Integral representation of the density matrix

The Hamiltonian of the spin-1/2 isotropic Heisenberg chain in a magnetic field $h$ is given as

$$H = J \sum_{j=1}^{L} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z) - \frac{h}{2} \sum_{j=1}^{L} \sigma_j^z, \quad (2.1)$$

where $\sigma_j^x$, $\sigma_j^y$, $\sigma_j^z$ are the Pauli matrices which act non-trivially on the $j$-th lattice site in a chain of length $L$. Here the periodic boundary condition
\[ \sigma_{j+L}^k = \sigma_j^k \] is assumed.

Let us introduce \( 2 \times 2 \) matrices:

\[
e^1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad e^2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad e'^1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad e'^2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (2.2)
\]

These matrices are embedded into the space \((\mathbb{C}^2)^\otimes L\) on which the Hamiltonian \((2.1)\) acts:

\[
e_{\alpha \beta}^\alpha = I^\otimes (j-1) \otimes e_{\beta}^\alpha \otimes I^\otimes (L-j), \quad (2.3)
\]

where \( I = e^1 + e^2, \alpha, \beta \in \{1, 2\} \) and \( j \in \{1, 2, \ldots, L\} \). The above Pauli matrices can be written in terms of these matrices: \( \sigma_j^x = e_{j}^1 + e_{j}^2, \sigma_j^y = ie_{j}^1 - ie_{j}^2, \sigma_j^z = e_{j}^1 - e_{j}^2 \). We also put \( \sigma_j^+ = e_{j}^2 \) and \( \sigma_j^- = e_{j}^1 \).

Göhmann, Klümper and Seel derived [1] an integral representation of the density matrix of the \( XXZ \) chain at finite temperature \( T \). The isotropic \( (XXX) \) limit of their formula is given as follows.

\[
< e_{1,\beta_1}^{\alpha_1} e_{2,\beta_2}^{\alpha_2} \cdots e_{m,\beta_m}^{\alpha_m} > = \lim_{L \to \infty} \frac{\text{Tr} e_{1,\beta_1}^{\alpha_1} e_{2,\beta_2}^{\alpha_2} \cdots e_{m,\beta_m}^{\alpha_m} e^{-H}}{\text{Tr} e^{-H}} = \prod_{j=1}^{[\alpha^+]} \int_C \frac{dy_j}{2\pi(1 + a(y_j))} (y_j - i)\bar{\alpha}_j^{-1} y_j^{-m - \bar{\alpha}_j} \\
\times \prod_{j=[\alpha^+]+1}^{m} \int_C \frac{dy_j}{2\pi(1 + a(y_j))} (y_j + i)\bar{\beta}_j^{-1} y_j^{-m - \bar{\beta}_j} \\
\times \prod_{1 \leq j \leq k \leq m} \left( \frac{\partial^{k-1}_{\xi} G(y_j, \xi)|_{\xi=0}}{(k-1)!} \right) \prod_{1 \leq j \leq k \leq m} (y_j - y_k - i) \quad (2.4)
\]

where \( a(v) \) and \( G(v, \xi) \) are solutions of the following integral equations.

\[
\log a(v) = -\frac{h}{T} + \frac{2J}{v(v+i)T} - \int_C dy \frac{\log(1 + a(y))}{\pi(1 + (v-y)^2)}, \quad (2.5)
\]

\[
G(v, \xi) = \frac{1}{(v-\xi)(v-\xi-i)} + \int_C dy \frac{1}{\pi(1 + (v-y)^2)} \frac{1}{1 + a(y)} G(y, \xi). \quad (2.6)
\]

Here \((\alpha_n)_n=1^m\) and \((\beta_n)_n=1^m\) are sequences of 1 or 2. We define the number of 1 in \((\alpha_n)_n=1^m\) as \([\alpha^+]\) and the position \( n \) of \( j \)-th 1 in \((\alpha_n)_n=1^m\) as \( \alpha_j^+ \): \( \alpha_j^+ = 1 \), \( 1 \leq \alpha_1^+ < \alpha_2^+ < \cdots < \alpha_{[\alpha^+]}^+ \leq m \). We also define the number of 2 in \((\beta_n)_n=1^m\) as \([\beta^-]\) and the position \( n \) of \( j \)-th 2 in \((\beta_n)_n=1^m\) as \( \beta_j^- \): \( \beta_j^- = 2 \),
1 \leq \beta^{-}_{1} < \beta^{-}_{2} < \cdots < \beta^{-}_{|\beta|} \leq m. \text{ We shall put } \tilde{\alpha}^{+}_{j} = \alpha^{+}_{|\beta|+j+1} \text{ for } j \in \{1, 2, \ldots, |\alpha^{+}|\} \text{ and } \beta^{-}_{j} = \beta^{-}_{|\alpha^{+}|+j} \text{ for } j \in \{|\alpha^{+}|+1, |\alpha^{+}|+2, \ldots, |\alpha^{+}|+|\beta^{+}|\}.
The contour \(C\) surrounds the real axis anti-clockwise manner. \(\mathfrak{a}(v)\) is defined as \(\mathfrak{a}(v) = 1/a(v)\). The emptiness formation probability is a special case of this density matrix element: \(P(m) = \langle e_{j_{1}}^{1}e_{j_{1}+1}^{1}\cdots e_{j_{m-1}}^{1} \rangle \). In this case, the multiple integral formula (2.4) reduces to the one in [3].

3 High temperature expansion

In this paper, we will calculate the HTE of the following two-point correlation functions for finite magnetic field \(h\):

\[
\langle \sigma_{j}^{\alpha}\sigma_{j+2}^{\alpha} \rangle = \langle (e_{j_{1}}^{1} - e_{j_{2}}^{1})(e_{j+1_{1}}^{1} + e_{j+1_{2}}^{1})(e_{j+2_{1}}^{1} - e_{j+2_{2}}^{1}) \rangle, \quad (3.1)
\]

\[
\langle \sigma_{j}^{\alpha}\sigma_{j+3}^{\alpha} \rangle = \langle (e_{j_{1}}^{1} - e_{j_{2}}^{1})(e_{j+1_{1}}^{1} + e_{j+1_{2}}^{1})(e_{j+2_{1}}^{1} + e_{j+2_{2}}^{1})(e_{j+3_{1}}^{1} - e_{j+3_{2}}^{1}) \rangle, \quad (3.2)
\]

\[
\langle \sigma_{j}^{+}\sigma_{j+2}^{-} \rangle = \langle e_{j_{1}}^{1}(e_{j+1_{1}}^{1} + e_{j+1_{2}}^{1})e_{j+2_{1}}^{1} \rangle. \quad (3.3)
\]

At \(h = 0\), one can express nearest neighbor and 2nd neighbor correlation functions in terms of \(P(2), P(3)\): \(\langle \sigma_{j}^{+}\sigma_{j+1}^{+} \rangle = 4P(2) - 1, \langle \sigma_{j}^{+}\sigma_{j+2}^{+} \rangle = 8(P(3) - P(2) + \frac{1}{8})\). Then we can immediately calculate the HTE of these correlation functions up to the order of 42 from the results in [14]. We can also calculate the HTE of \(\langle \sigma_{j}^{+}\sigma_{j+2}^{-} \rangle\) up to the order of 42 from the relation \(\langle \sigma_{j}^{+}\sigma_{j+2}^{-} \rangle = \frac{1}{2} \langle \sigma_{j}^{+}\sigma_{j+2}^{+} \rangle\) which holds for isotropic model (XXZ-model) at \(h = 0\). Moreover one can calculate the nearest neighbor correlation functions by taking the derivative of the free energy of the XXZ-chain with respect to the anisotropy parameter. On the other hand, \(\langle \sigma_{j}^{+}\sigma_{j+3}^{-} \rangle\) can not be expressed only in terms of \(P(m)\) even at \(h = 0\).

At first, we will calculate the HTE of \(a(v)\) from the NLIE (2.5). Note that this calculation is similar to the one for the HTE for the free energy [9]. We assume the following expansion for small \(|J/T|\):

\[
a(v) = \exp \left( \sum_{k=1}^{\infty} a_{k}(v) \left( \frac{J}{T} \right)^{k} \right) = 1 + a_{1}(v)\frac{J}{T} + \left( \frac{a_{1}(v)^{2}}{2} + a_{2}(v) \right) \left( \frac{J}{T} \right)^{2} + \left( \frac{a_{1}(v)^{3}}{6} + a_{1}(v)a_{2}(v) + a_{3}(v) \right) \left( \frac{J}{T} \right)^{3} + \left( \frac{a_{1}(v)^{4}}{24} + \frac{a_{1}(v)^{2}a_{2}(v)}{2} + \frac{a_{2}(v)^{2}}{2} + a_{1}(v)a_{3}(v) + a_{4}(v) \right) \left( \frac{J}{T} \right)^{4} + \cdots . \quad (3.4)
\]

Substituting (3.4) into (2.5), and comparing coefficients of \((J/T)^{m}\) on both
sides, we obtain the following integral equation for each $m \ (m \in \mathbb{Z}_{\geq 1})$:

$$a_m(v) = \left( -\frac{h}{J} + \frac{2}{v(v+i)} \right) \delta_{m,1} - \int_{C} \frac{dy \ a_m(y)}{\pi} + A_m(y), \quad (3.5)$$

where $A_m(y)$ is made of $\{a_k(y)\}_{k=1}^{m-1}$:

$$A_1(y) = 0, \quad A_2(y) = \frac{a_1(y)^2}{8}, \quad A_3(y) = \frac{a_1(y)a_2(y)}{4},$$

$$A_4(y) = -\frac{a_1(y)^4 + 24a_2(y)^2 + 48a_1(y)a_3(y)}{192}, \ldots. \quad (3.6)$$

We can solve (3.5) recursively. The first few terms of $\{a_m(v)\}$ are

$$a_1(v) = -\frac{h}{J} - \frac{2i}{v(1+v^2)}, \quad a_2(v) = \frac{h}{J(1+v^2)} + \frac{2iv}{(1+v^2)^2},$$

$$a_3(v) = -\frac{h}{J(1+v^2)},$$

$$a_4(v) = -\frac{2iv(3+3v^2+2v^4)}{3(1+v^2)^4} - \frac{h(1-3v^2)}{3J(1+v^2)^3} - \frac{ih^2v}{2J^2(1+v^2)^2} - \frac{h^3}{12J^3(1+v^2)}$$

$$\ldots. \quad (3.7)$$

One sees that only $a_1(v)$ has a pole at the origin. One can also solve the integral equation (2.6) based on the results of (2.5). We assume the following expansion for small $|J/T|$:

$$G(v, \xi) = \sum_{k=0}^{\infty} g_k(v, \xi) \left( \frac{J}{T} \right)^k. \quad (3.8)$$

Substituting (3.8) into (2.6), we can obtain the coefficients. The first few
terms of \( \{ g_k(v, \xi) \} \) are

\[
\begin{align*}
  g_0(v, \xi) &= \frac{-i}{(1 + (v - \xi)^2)(v - \xi)}, \\
  g_1(v, \xi) &= \frac{i(2v - \xi)}{(1 + v^2)(1 + (v - \xi)^2)(1 + \xi^2)} + \frac{h}{2J(1 + (v - \xi)^2)}, \\
  g_2(v, \xi) &= -\frac{i(2v - \xi)\xi^2}{(1 + v^2)(1 + (v - \xi)^2)(1 + \xi^2)} - \frac{h(2 + 2v^2 - 2v\xi + \xi^2)}{2J(1 + v^2)(1 + (v - \xi)^2)(1 + \xi^2)}, \\
  g_3(v, \xi) &= -i\left( (6\xi^2 + 8) v^5 - \xi \left( 9\xi^2 + 10 \right) v^4 + 4 \left( 2\xi^2 + 3 \right) v^3 + \xi \left( 3\xi^4 - 4\xi^2 - 9 \right) v^2 + 2 \left( 4\xi^4 + 9\xi^2 + 6 \right) v - \xi \left( \xi^4 + 3\xi^2 + 3 \right) \right) \\
  &\quad + \frac{h}{2J(v^2 + 1)} \left( \left( v - \xi \right)^2 + 1 \right) \left( \xi^2 + 3 \right) \\
  &\quad + \frac{h^2}{4J^2} \left( i\xi - 2iv \right) \left( v - \xi \right)^2 + \frac{h^3}{24J^3} \left( v - \xi \right)^2 + 1. 
\end{align*}
\]

(3.9)

One see that only \( g_0(v, \xi) \) has a pole at \( v = \xi \). Taking note on the above results and substituting (3.4) and (3.8) into (2.4), we can calculate the coefficients of the HTE for the density matrix in a finite magnetic field \( h \) only by taking residues at the origin. Then we can calculate the HTE of the two point functions (3.1)-(3.3) by using the result on the HTE of matrix elements of the density matrix. For example, the HTE of a 3rd neighbor correlation function at \( h = 0 \) up to the order of 25 is given as follows:

\[
< \sigma_j \sigma_{j+3} > = -t^3 - t^4 + \frac{58t^5}{15} + \frac{382t^6}{45} - \frac{545t^7}{63} - \frac{14473t^8}{315} - \frac{3227t^9}{405} + \frac{2715697t^{10}}{14175} + \frac{34762571t^{11}}{405659182t^{14}} - \frac{31700839t^{12}}{63851285} - \frac{51975}{1373907665967541t^{15}} + \frac{1774892665829t^{16}}{63851285} - \frac{868725}{10854718875} - \frac{32564156625}{184007137948420708921} + \frac{16874153875}{12993098493375} - \frac{94567556978993784629t^{22}}{714620417135625} - \frac{16436269594119375}{4135206247498584771500543t^{25}} + \frac{52830228665525265625}{4930880872358125} - \frac{10941168707397851825299t^{23}}{25160268799380101833103t^{24}} + \frac{105157865665625}{21359281025},
\]

(3.10)

where we put \( t = J/T \). We also calculated the HTE of \( < \sigma_j \sigma_{j+2} > \) for finite magnetic fields \( h = 2, 4, 6, 8 \) up to the order of 30; \( < \sigma_j \sigma_{j+3} > \) for
$h = 2, 4, 6, 8$ up to the order of 20; $\langle \sigma_j^+ \sigma_{j+2}^- \rangle$ for $h = 2, 4, 6, 8$ up to the order of 30. In [16, 17], the HTE of correlation functions for zero magnetic field were calculated up to the order of 19 by other method. It is remarkable that we can also treat nonzero magnetic field case and the orders of our HTE are higher than the ones in [16, 17].

We have plotted the Padé approximations of the HTE of these correlation functions for finite magnetic fields $h$ in Figures 1-5. Once we introduce the HTE, we can also consider $J < 0$ case by analytic continuation, though original multiple integral formula (2.4) was defined for $J > 0$ case. We have also plotted quantum Monte Carlo simulation (QMC) data by Shiroishi [18] based on the open source software in the ALPS project [19, 20]. The system size of the simulations is $L = 128$. Our HTE results agree well with these QMC data except in the very low temperature regions. At least in the region where the Padé approximation seems to converge, $\langle \sigma_j^+ \sigma_{j+2}^- \rangle$ for $J > 0$ at $h = 0$ and for $J < 0$, $\langle \sigma_j^+ \sigma_{j+3}^- \rangle$ for $J < 0$ and $\langle \sigma_j^+ \sigma_{j+2}^- \rangle$ at $h = 0$ monotonously decrease with respect to temperature (here we omit a figure of $\langle \sigma_j^+ \sigma_{j+2}^- \rangle$ for $J < 0$); $\langle \sigma_j^+ \sigma_{j+3}^- \rangle$ for $J > 0$ at $h = 0$ monotonously increases with respect to temperature. When $h > 0$ in figures [12,15] peaks appear at non-trivial temperatures.

4 Concluding remarks

In this paper, we have evaluated the multiple integral formula of the density matrix by using the HTE method, and thereby obtained the HTE of several two point correlation functions. Together with our previous paper [14] on $P(m)$, we recognized that the HTE method is efficient to evaluate the multiple integral formulae of correlation functions [1]-[3]. In [23], the multiple integral formula (2.4) has been reduced to finite sums over products of single integrals for short segments of length 2 and 3. If a similar reduction is done for length 4, one will be able to calculate the HTE whose order is higher than the one in this paper.

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Figure 1: Temperature $T$ dependence of $\langle \sigma_j^z \sigma_{j+2}^z \rangle$ for $J > 0$ with a magnetic field $h$. We have plotted the Padé approximations of order $[21, 21]$ for $h = 0$ and $[15, 15]$ for $h = 2, 4, 6, 8$ ([n,d] means that the numerator is a degree $n$ polynomial of $J/T$ and the denominator is a degree $d$ polynomial of $J/T$). An exact value of $\langle \sigma_j^z \sigma_{j+2}^z \rangle$ at $(T, h) = (0, 0)$ was calculated in [21].
Figure 2: Temperature $T$ dependence of $\langle \sigma_j^z \sigma_{j+3}^z \rangle$ for $J > 0$ with a magnetic field $h$. We have plotted the Padé approximations of order $[12, 13]$ for $h = 0$ and $[10, 10]$ for $h = 2, 4, 6, 8$. An exact value of $\langle S_j^z S_{j+3}^z \rangle = \frac{1}{4} < \sigma_j^z \sigma_{j+3}^z >$ at $(T, h) = (0, 0)$ was calculated in [22].
Figure 3: Temperature $T$ dependence of $\langle \sigma_j^z \sigma_{j+3}^z \rangle$ for $J < 0$ with a magnetic field $h$. We have plotted the Padé approximations of order $[12, 13]$ for $h = 0$ and $[10, 10]$ for $h = 2, 4, 6, 8$. 
Figure 4: Temperature $T$ dependence of $\langle \sigma_{j}^{+}\sigma_{j+2}^{-}\rangle$ for $J > 0$ with a magnetic field $h$. We have plotted the Padé approximations of order [21, 21] for $h = 0$ and [15, 15] for $h = 2, 4, 6, 8$. An exact value of $\langle \sigma_{j}^{z}\sigma_{j+2}^{z}\rangle = 2 \langle \sigma_{j}^{+}\sigma_{j+2}^{-}\rangle$ at $(T, h) = (0, 0)$ was calculated in [21].
Figure 5: Temperature $T$ dependence of $\langle \sigma_j^{+}\sigma_{j+2}^{-}\rangle$ for $J < 0$ with a magnetic field $h$. We have plotted the Padé approximations of order $[21,21]$ for $h = 0$, $[15,15]$ for $h = 2, 4, 6$ and $[14,16]$ for $h = 8$. 
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