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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 third neighbor correlation function $\langle \sigma_j^z \sigma_{j+3}^z \rangle$ 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–L370, condmat/0502569.] to more general correlation functions.

Keywords: Correlation function; Density matrix; High temperature expansion; Nonlinear integral equation; Quantum transfer matrix

1. Introduction

Göhmann, et al. [1] derived (see also Refs. [2–5]) a multiple integral formula of matrix elements of a density matrix of a finite segment of arbitrary length m of the anti-ferromagnetic spin $\frac{1}{2}$ *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 [11–13] to finite temperature case. This is a fundamental quantity since thermal average of any operators acting nontrivially 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 nontrivial 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

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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 $\frac{1}{2}$ 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 [1]. 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 third 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-$\frac{1}{2}$ isotropic Heisenberg chain in a magnetic field h is given as

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

where σ_j^x, σ_j^y, σ_j^z are the Pauli matrices which act nontrivially on the jth 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 2×2 matrices:

$$e_1^1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad e_1^2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad e_2^1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad e_2^2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{2.2}$$

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

$$e_{j\beta}^{\alpha} = I^{\otimes(j-1)} \otimes e_\beta^\alpha \otimes I^{\otimes(L-j)}, \tag{2.3}$$

where $I = e_1^1 + e_2^2$, $\alpha, \beta \in \{1, 2\}$ and $j \in \{1, 2, \ldots, L\}$. The above Pauli matrices can be written in terms of these matrices: $\sigma_j^x = e_{j2}^{1} + e_{j1}^{2}$, $\sigma_j^y = \mathrm{i}e_{j2}^{1} - \mathrm{i}e_{j1}^{2}$, $\sigma_j^z = e_{j1}^{1} - e_{j2}^{2}$. We also put $\sigma_j^+ = e_{j1}^{2}$ and $\sigma_j^- = e_{j2}^{1}$.

Göhmann, et al. [1] derived 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:

$$\begin{aligned}
\langle e_{1\beta_1}^{\alpha_1} e_{2\beta_2}^{\alpha_2} \cdots e_{m\beta_m}^{\alpha_m}\rangle &= \lim_{L\to\infty} \frac{\mathrm{Tr}\, e_{1\beta_1}^{\alpha_1} e_{2\beta_2}^{\alpha_2} \cdots e_{m\beta_m}^{\alpha_m} e^{-H/T}}{\mathrm{Tr}\, e^{-H/T}} \\
&= \prod_{j=1}^{|\alpha^+|} \int_C \frac{\mathrm{d}y_j}{2\pi(1+\mathfrak{a}(y_j))} (y_j - \mathrm{i})^{\widetilde{\alpha_j^+}-1} y_j^{m-\widetilde{\alpha_j^+}} \\
&\quad \times \prod_{j=|\alpha^+|+1}^{m} \int_C \frac{\mathrm{d}y_j}{2\pi(1+\overline{\mathfrak{a}}(y_j))} (y_j + \mathrm{i})^{\widetilde{\beta_j^-}-1} y_j^{m-\widetilde{\beta_j^-}} \\
&\quad \times \det_{1\leqslant j,k\leqslant m}\left(\frac{\partial_\xi^{(k-1)} G(y_j,\xi)|_{\xi=0}}{(k-1)!}\right) \frac{1}{\prod_{1\leqslant j<k\leqslant m}(y_j - y_k - \mathrm{i})},
\end{aligned} \tag{2.4}$$

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

$$\log\mathfrak{a}(v) = -\frac{h}{T} + \frac{2J}{v(v+i)T} - \int_C \frac{\mathrm{d}y}{\pi} \frac{\log(1+\mathfrak{a}(y))}{1+(v-y)^2}, \tag{2.5}$$

$$G(v,\xi) = -\frac{1}{(v-\xi)(v-\xi-i)} + \int_C \frac{\mathrm{d}y}{\pi} \frac{1}{1+(v-y)^2} \frac{G(y,\xi)}{1+\mathfrak{a}(y)}. \tag{2.6}$$

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 jth 1 in $(\alpha_n)_{n=1}^m$ as α_j^+: $\alpha_{\alpha_j^+} = 1$, $1 \leqslant \alpha_1^+ < \alpha_2^+ < \cdots < \alpha_{|\alpha^+|}^+ \leqslant m$. We also define the number of 2 in $(\beta_n)_{n=1}^m$ as $|\beta^-|$ and the position n of jth 2 in $(\beta_n)_{n=1}^m$ as β_j^-: $\beta_{\beta_j^-} = 2$, $1 \leqslant \beta_1^- < \beta_2^- < \cdots < \beta_{|\beta^-|}^- \leqslant m$. We shall put $\widetilde{\alpha_j^+} = \alpha_{|\alpha^+|-j+1}^+$ for $j \in \{1, 2, \ldots, |\alpha^+|\}$ and $\widetilde{\beta_j^-} = \beta_{j-|\alpha^+|}^-$ for $j \in \{|\alpha^+|+1, |\alpha^+|+2, \ldots, |\alpha^+|+|\beta^-|\}$. The contour C surrounds