High temperature expansion of emptiness formation probability for isotropic Heisenberg chain

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Recently, Göhmann, Klümper and Seel have derived novel integral formulas for the correlation functions of the spin-1/2 Heisenberg chain at finite temperature. We have found that the high temperature expansion (HTE) technique can be effectively applied to evaluate these integral formulas. Actually, as for the emptiness formation probability \( P(n) \) of the isotropic Heisenberg chain, we have found a general formula of the HTE for \( P(n) \) with arbitrary \( n \in \mathbb{Z}_{\geq 2} \) up to \( O((J/T)^4) \). If we fix a magnetic field to a certain value, we can calculate the HTE to much higher order. For example, the order up to \( O((J/T)^{12}) \) has been achieved in the case of \( P(3) \) when \( h = 0 \). We have compared these HTE results with the data by Quantum Monte Carlo simulations. They exhibit excellent agreements.

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The spin-1/2 Heisenberg chain has been one of the most fundamental models in the study of the low dimensional magnetism, partially because it can be solved exactly by Bethe ansatz. In fact, many physical quantities of the model have been evaluated exactly even at finite temperature \(^1\). However, they are usually the bulk properties, which may be derived directly from the free-energy of the system. The exact evaluation of the correlation functions at finite temperature, on the other hand, has remained to be a much more difficult problem. Actually, as for the emptiness formation probability \( P(n) \) an additional auxiliary function \( \xi \) has been introduced in \(^2\) and studied further, for example, in \(^3\)\(^4\)\(^5\). Recently Göhmann, Klümper and Seel obtained \(^11\)\(^12\) the multiple integral formulas of the EFP at finite temperature as

\[
P(n) = \frac{\prod_{j=1}^n dy_j}{\prod_{j=1}^n 2\pi(1 + a(y_j))} \left| \frac{\det_{1 \leq j, k \leq n} \left( \frac{\partial_{\xi}^{k-1} G(y_j, \xi) |_{\xi=0}}{(k-1)!} \right)}{\prod_{1 \leq j < k \leq n} (y_j - y_k + i)} \right|,
\]

where functions \( a(v) \) and \( G(v, \xi) \) are solutions of the NLIE:

\[
\log a(v) = -\frac{J}{T} + \frac{2J}{v(i + T)} - \int_C \frac{dy \log(1 + a(y))}{\pi}, \quad (4)
\]

\[
G(v, \xi) = -\frac{1}{(v - \xi)(v - \xi - i)} + \int_C \frac{dy}{\pi(1 + (v - y)^2)} \frac{1}{1 + a(y)} G(y, \xi), \quad (5)
\]

The Hamiltonian of the spin-1/2 isotropic Heisenberg chain in a magnetic field \( h \) is defined by

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

where \( \sigma_j^k (k = x, y, z) \) are the Pauli matrices \( \sigma^k \) acting non-trivially on the \( j \)-th site of the chain of length \( L \). Here we adopt the periodic boundary condition \( \sigma_{j+L} = \sigma_j \). In this letter, we mainly consider a special correlation function called the emptiness formation probability (EFP) \( P(n) \), which is the probability of \( n \) adjacent spins being aligned upward:

\[
P(n) = \frac{\Tr e^{-\frac{H}{T} \prod_{j=1}^n \frac{1+\sigma_j^z}{2}}}{\Tr e^{-\frac{H}{T}}}. \quad (2)
\]

At zero temperature \( T = 0 \), it was introduced in \(^2\) and studied further, for example, in \(^3\)\(^4\)\(^5\). Recently Göhmann, Klümper and Seel obtained \(^11\)\(^12\) the multiple integral formulas of the EFP at finite temperature as

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\]
Here the contour \( C \) surrounds the real axis anti-clockwise manner.

First, let us calculate the HTE of \( a(v) \) from the NLIE. This is done by a similar procedure in \([17]\), where a certain order of the HTE for the free-energy was calculated from a NLIE. We assume the following expansion for small \( J/T \),

\[
a(v) = \exp \left( \sum_{k=1}^{\infty} a_k(v) \left( \frac{J}{T} \right)^k \right).
\]

Substituting (6) into (4), and comparing coefficients of \( (J/T)^m \) on both sides, we obtain an integral equation over \( \{a_k(v)\}_{k=1}^{\infty} \) for each \( m \ (m \in \mathbb{Z}_{\geq 1}) \). As the resultant integral equation is linear with respect to \( a_m(v) \), we can solve it recursively. For example, we obtain

\[
a_1(v) = -\frac{h}{J} - \frac{2i}{v(1 + v^2)},
\]

\[
a_2(v) = \frac{h}{J(1 + v^2)} + \frac{2iv}{(1 + v^2)^2},
\]

\[
a_3(v) = -\frac{h}{J(1 + v^2)}.
\]

Note that only \( a_1(v) \) has a pole at the origin. Next let us consider the integral equation (5). We assume the following expansion for small \( J/T \),

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

In a similar way, we can determine the coefficients \( g_n(v, \xi) \) successively by using the results on (5). For example, we obtain

\[
g_0(v, \xi) = \frac{-i}{(1 + (v - \xi)^2)(v - \xi)},
\]

\[
g_1(v, \xi) = \frac{h}{(1 + v^2)(1 + (v - \xi)^2)(1 + \xi^2)}
\]

\[
+ \frac{2ih}{J(1 + (v - \xi)^2)};
\]

\[
g_2(v, \xi) = \frac{-i(2v - \xi)^2}{(1 + v^2)(1 + (v - \xi)^2)(1 + \xi^2)}
\]

\[
- \frac{h(2 + 2v^2 - 2v \xi + \xi^2)}{2J(1 + v^2)(1 + (v - \xi)^2)(1 + \xi^2)}.
\]

Note that only \( g_0(v, \xi) \) has a pole at \( v = \xi \). Finally, substituting (5) and (6) into (5), we can obtain the HTE of \( P(n) \). Unexpectedly we have found that we only have to calculate residues at the origin. In fact, in this way, we could calculate the HTE of the \( P(n) \) for small \( n \ (n \in \{2, 3, 4, 5, 6\}) \). The result up to the order \( O((J/T)^4) \) is compactly presented as

\[
P(n) = \frac{1}{2^n} + \frac{-2J(-1 + n) + hn}{2^{1+n}T} + \left\{ 4J^2(-4 + n)(-1 + n) + h^2(-1 + n)n \right. \\
- 4hJ(2 + (-1 + n)n)}{2^{3+n}T^2}
\]

\[
+ \left\{ 12hJ^2(-2 + n)^2(-1 + n) + h^3(-3 + n)n^2 \right. \\
- 8J^3(-24 + (-9 + n)(-3 + n)n) \\
- 6h^2J(1 - n)(2 + (-1 + n)n)}{1 \cdot 3 \cdot 2^{4+n}T^3}
\]

\[
+ \left\{ 24h^2J^2(-2 - n)^2(-1 + n)^2 \\
+ 16J^4(-5 + n)(-32 + n(26 + (-17 + n)n)) \\
+ h^4n(2 + n(3 - 6 + n)n) \\
- 32hJ^3(24 + (-9 + n)n(6 - (3 + n)n)) \\
- 8h^3J(-4 + (-4 + n)n(3 + n^2)) \right\} \frac{1}{3 \cdot 2^{7+n}T^4} + O \left( \left( \frac{J}{T} \right)^5 \right).
\]

We observe that \( P(n) \) has the following form

\[
P(n) = \frac{1}{2^n} \sum_{m=0}^{\infty} \sum_{m=0}^{\infty} \frac{1}{m!} \left( \sum_{k=0}^{m} p_{m,k}(n) \left( \frac{h}{J} \right)^k \right) \left( \frac{J}{2T} \right)^m,
\]

where \( p_{0,0}(n) = 1 \) and \( p_{m,k}(n) \) for \( m \in \mathbb{Z}_{\geq 1} \) are functions of \( n \), which are independent of \( J \), \( h \), and \( T \). If we admit that \( p_{m,k}(n) \) is a polynomial of \( n \) whose degree is at most \( m \), our formula (10) is also valid for any \( n \in \mathbb{Z}_{\geq 2} \) as the \( m \)-th order polynomial is determined by distinct \( m + 1 \) points.

Next we fix the magnetic field \( h \) to certain values and calculate the HTE to much higher order. Then we have succeeded in obtaining coefficients of \( P(3) \) up to the order \( O((J/T)^4) \) in the case of \( h = 0 \). For a finite \( h \), we can calculate them at least up to the order \( O((J/T)^6) \). It will not be easy to obtain HTE coefficients, in particular under the magnetic field, to such a high order by other method except for the free models. We list some of our results on \( h = 0 \) case in Table II.

![FIG. 1: \( P(n) \) for \( J > 0 \) at \( h = 0 \).](image-url)
Moreover we have applied the Padé approximation to our HTE and plot the results in Fig. 1-Fig. 5. Note that although the formula (8) was originally derived for $J > 0$ case, our HTE results can be analytically continued to $J < 0$ case. For comparison, we have also performed Quantum Monte Carlo simulation (QMC) using recent open source softwares in ALPS project [20]. Especially we have chosen the SSE algorithm [21] so as to treat finite magnetic field cases. We have performed the simulations with the system size $L = 128$. In Fig. 1-Fig. 5, these QMC data are represented by solid triangles, which show excellent agreements with the HTE results. Discrepancy appears only in the very low temperature regions, where even the Padé approximation of the HTE ceases to converge. We omit these apparent deviations of the Padé approximation in Fig. 2. We remark that we have also tested the validity of our general formula (10) up to $n = 20$.

In the case of $J > 0$ and $h = 0$, we see that $P(n)$ monotonously increases as the temperature increases. On the other hand, it decreases monotonously for $J < 0$. In this case we have found $P(n) \to 1/(n + 1)$ as $T \to 0$. Another interesting observation in Fig. 3 is that, when $J > 0$, a peak appears for positive values of the magnetic field. Its position moves from $T = \infty$ to 0 as $h$ increases. For example, the peak position $T^{\max}$ and the peak $P(3)^{\max}$ are given by $(h/J, T^{\max}/J, P(3)^{\max}) = (2, 12.030, 0.13015), (4, 3.7467, 0.18973), (6, 1.6904, 0.33416)$, respectively. Note that in this case, the critical field is $h_c = 8J$ at $T = 0$, where all the spins are directed upward.

In conclusion we have found that our HTE method is very powerful to evaluate the integral formula for $P(n)$ at finite temperature. As an alternative way, it may be possible to solve the NLIEs (1) and (5) numerically and perform numerical integration for the multiple integrals in (8). We have tried it, but found it hard to get reliable numerical results even for $P(3)$.

It is straightforward to generalize the results in this letter to more general correlation functions. Actually as for the nearest and the next-nearest-neighbor correlation functions for $h = 0$, we can immediately calculate their HTEs from our results through the relations $\langle S_j^z S_{j+1}^z \rangle = P(2) - 1/2, \langle S_j^z S_{j+2}^z \rangle = 2P(3) - P(2) + 1/8$, from which we can obtain the coefficients whose order is higher than the ones by other method [12]. We can evaluate the HTE for other complicated correlation functions based on the multiple integral formula on the density matrix of the $XXZ$ chain at finite temperatures [13]. We will report on details in the forthcoming paper [22].

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TABLE I: Series coefficients $p_k(n)$ for the high temperature expansion of $P(n) = \sum_k p_k(n)(\frac{1}{T})^k$ at $h = 0$.

| $k$ | $p_k(3)$ | $p_k(4)$ | $p_k(5)$ |
|-----|---------|---------|---------|
| 0   | $\frac{1}{4}$ | $\frac{1}{6}$ | $\frac{1}{8}$ |
| 1   | $\frac{1}{2}$ | $\frac{1}{3}$ | $\frac{1}{5}$ |
| 2   | $\frac{1}{4}$ | $\frac{1}{5}$ | $\frac{1}{7}$ |
| 3   | $\frac{1}{6}$ | $\frac{1}{7}$ | $\frac{1}{9}$ |
| 4   | $\frac{1}{8}$ | $\frac{1}{9}$ | $\frac{1}{11}$ |
| 5   | $\frac{1}{10}$ | $\frac{1}{11}$ | $\frac{1}{13}$ |
| 6   | $\frac{1}{12}$ | $\frac{1}{13}$ | $\frac{1}{15}$ |
| 7   | $\frac{1}{14}$ | $\frac{1}{15}$ | $\frac{1}{17}$ |
| 8   | $\frac{1}{16}$ | $\frac{1}{17}$ | $\frac{1}{19}$ |
| 9   | $\frac{1}{18}$ | $\frac{1}{19}$ | $\frac{1}{21}$ |
| 10  | $\frac{1}{20}$ | $\frac{1}{21}$ | $\frac{1}{23}$ |

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