Quantum Correlations and Number Theory

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Abstract

We study spin-1/2 Heisenberg \textit{XXX} antiferromagnet. The spectrum of the Hamiltonian was found by Hans Bethe in 1931, [1]. We study the probability of formation of ferromagnetic string in the antiferromagnetic ground state, which we call emptiness formation probability \( P(n) \). This is the most fundamental correlation function. We prove that for the short strings it can be expressed in terms of the Riemann zeta function with odd arguments, logarithm \( \ln 2 \) and rational coefficients. This adds yet another link between statistical mechanics and number theory. We have obtained an analytical formula for \( P(5) \) for the first time.

We have also calculated \( P(n) \) numerically by the Density Matrix Renormalization Group. The results agree quite well with the analytical ones. Furthermore we study asymptotic behavior of \( P(n) \) at finite temperature by Quantum Monte-Carlo simulation. It also agrees with our previous analytical results.

1 Introduction

Recently the considerable progress has been achieved for the exact calculation of correlation functions in the spin-1/2 Heisenberg \textit{XXZ} chain [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]. Hans Bethe discovered his Ansatz, while diagonalising \textit{XXX} Hamiltonian. The most important features of exactly solvable models, like two-body reducibility of dynamics were first discovered for this model. We believe that the antiferromagnetic Heisenberg \textit{XXX} chain is one of the most fundamental exactly solvable models. Recently we developed a new method of evaluation of the multi-integral representation of correlation functions [10, 11].

We study the most fundamental correlation function of the model, which we call emptiness formation probability \( P(n) \). We shall abbreviate it to EFP. It was first introduced in [4]

\[
P(n) = \langle \text{GS} | \prod_{j=1}^{n} P_j | \text{GS} \rangle, \tag{1.1}
\]

where \( P_j = S_j^z + \frac{1}{2} \) is the projector on the state with the spin up in the \( j \)-th lattice site. \(|\text{GS}\rangle \) is the antiferromagnetic ground state in the thermodynamic limit constructed by Hulthén [13]. \( P(n) \) is a probability of formation of a ferromagnetic string of length \( n \) in \(|\text{GS}\rangle\).

The Hamiltonian of the Heisenberg \textit{XXX} chain is given by

\[
H = J \sum_{j=1}^{N} \left( S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z - \frac{1}{4} \right), \tag{1.2}
\]
where the coupling constant \( J \) is positive for the antiferromagnet.

In ref. \([10, 11]\), we wrote the Hamiltonian \((1.2)\) in terms of the Pauli matrices. It corresponds to \( J = 4 \).

First cases \( P(3) \) and \( P(4) \) were calculated by means of the multi-integral representation in \([14, 15]\). In this paper, we present a new analytic formula for \( P(5) \)

\[
P(5) = \frac{1}{6} - \frac{10}{3} \ln 2 + \frac{281}{24} \zeta(3) - \frac{45}{2} \ln 2 \cdot \zeta(3) - \frac{489}{16} \zeta(3)^2 \\
- \frac{6775}{192} \zeta(5) + \frac{1225}{6} \ln 2 \cdot \zeta(5) - \frac{425}{64} \zeta(3) \cdot \zeta(5) - \frac{12125}{256} \zeta(5)^2 \\
+ \frac{6223}{512} \zeta(7) - \frac{11515}{64} \ln 2 \cdot \zeta(7) + \frac{42777}{512} \zeta(3) \cdot \zeta(7)
\]

\[
= 2.011725953 \times 10^{-6}.
\]

(1.3)

where \( \zeta(s) \) is the Riemann zeta function

\[
\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^n}, \quad \text{for } \Re(s) > 1.
\]

(1.4)

\( P(5) \) is expressed in terms of \( \ln 2, \zeta(3), \zeta(5) \) and \( \zeta(7) \) with rational coefficients. In fact, it was conjectured \([11]\):

"\( P(n) \) is always expressed in terms of logarithm \( \ln 2 \), Riemann zeta functions \( \zeta(2k + 1) \) with odd argument and rational coefficients."

This means that all values of \( P(n) \) are different transcendental numbers \([4]\).

For comparison, let us list previous results for \( P(n) \).

\[
P(1) = \frac{1}{2} = 0.5, \quad (1.5)
\]

\[
P(2) = \frac{1}{3} = 0.33333333, \quad (1.6)
\]

\[
P(3) = \frac{1}{4} - \frac{3}{8} \zeta(3) = 0.007624158, \quad (1.7)
\]

\[
P(4) = \frac{1}{5} - \frac{2 \ln 2 + \frac{173}{60} \zeta(3) - \frac{11}{6} \ln 2 \cdot \zeta(3) - \frac{51}{80} \zeta(3)}{24} \\
- \frac{55}{24} \zeta(5) + \frac{85}{24} \ln 2 \cdot \zeta(5) = 0.000206270. \quad (1.8)
\]

Let us mention that in contrast with \( P(1), P(2), P(3) \) [which do not contain non-linear terms of the Riemann zeta function] the values \( P(4) \) and \( P(5) \) do contain non-linear terms in Riemann zeta function. It might be instructive to express formulas \((1.3), (1.9)\) for \( P(5) \) and \( P(4) \) in a linear form by introducing the multiple zeta values \([13]\)

\[
\zeta(k_1, k_2, \ldots, k_m) = \sum_{n_1 > n_2 > \ldots > n_m > 0} n_1^{-k_1} n_2^{-k_2} \ldots n_m^{-k_m}. \quad (1.9)
\]

The length (or depth) of this multiple zeta value is equal to \( m \) and the level (or weight) is equal to \( k_1 + k_2 + \ldots + k_m \). The result looks as follows:

\[
P(4) = \frac{1}{5} - \frac{2 \ln 2 + \frac{173}{60} \zeta(3) - \frac{11}{6} \ln 2 \cdot \zeta(3) - \frac{55}{24} \zeta(5) + \frac{85}{24} \ln 2 \cdot \zeta(5)}{24} \\
- \frac{51}{10} \zeta(3,3) + \frac{153}{80} \zeta(4,2), \quad (1.10)
\]

\[
P(5) = \frac{1}{6} - \frac{10}{3} \ln 2 + \frac{281}{24} \zeta(3) - \frac{45}{2} \ln 2 \cdot \zeta(3) - \frac{6775}{192} \zeta(5) \\
+ \frac{1225}{6} \ln 2 \cdot \zeta(5) + \frac{6223}{256} \zeta(7) - \frac{11515}{64} \ln 2 \cdot \zeta(7) \\
- \frac{489}{2} \zeta(3,3) + \frac{1467}{16} \zeta(4,2) - \frac{12495}{128} \zeta(4,4) - \frac{85}{64} \zeta(5,3) - \frac{425}{128} \zeta(6,2) \\
+ \frac{487037}{512} \zeta(5,5) + \frac{584425}{1024} \zeta(6,4) + \frac{596647}{1024} \zeta(7,3) + \frac{42777}{1024} \zeta(8,2). \quad (1.11)
\]

Here we used the following identities

\[
\zeta(3)^2 = 8 \zeta(3,3) - 3 \zeta(4,2),
\]

\[
\zeta(3) \cdot \zeta(5) = \frac{147}{10} \zeta(4,4) + \frac{1}{5} \zeta(5,3) + \frac{1}{2} \zeta(6,2),
\]

\[
\zeta(5)^2 = 22 \zeta(5,5) + 10 \zeta(6,4) + 10 \zeta(7,3),
\]

\[
\zeta(3) \cdot \zeta(7) = \frac{167}{7} \zeta(5,5) + \frac{25}{2} \zeta(6,4) + \frac{177}{14} \zeta(7,3) + \frac{1}{2} \zeta(8,2). \quad (1.12)
\]
These identities can be derived using the recurreent relations (4.1), (4.5),...,(4.7) of ref. [10]. Let us note that the Drinfeld’s associator is also related to multiple zeta values in a linear way [12].

Since, ln2 in formulae above looks somehow isolated, we believe that it seems to be more appropriate to express P(n) in terms of the alternating zeta series (the value of polylogarithm at root of unity)

$$\zeta_a(s) = \sum_{n>0} \frac{(-1)^{n-1}}{n^s} = -\text{Li}_s(-1)$$  \hspace{1cm} (1.13)

Here Li_a(x) is the polylogarithm. The alternating zeta series is related to the Riemann zeta function as follows

$$\zeta(s) = \frac{1}{1 - 2^{1-s}} \zeta_a(s)$$  \hspace{1cm} (1.14)

This formula is valid for $s \neq 1$. In contrast with the zeta function [which has the pole when $s \to 1$], the alternating zeta has a limit as $s \to 1$

$$\zeta_a(1) = \ln 2$$  \hspace{1cm} (1.15)

Using the formulae (1.3),...,(1.8), (1.14) and (1.13), one can get the five first values of $P(n)$ expressed via the alternating zeta series

$$
\begin{align*}
P(1) &= \frac{1}{2}, \\
P(2) &= \frac{1}{3} \{1 - \zeta_a(1)\}, \\
P(3) &= \frac{1}{4} \{1 - 4\zeta_a(1) + 2\zeta(3)\}, \\
P(4) &= \frac{1}{5} \{1 - 10\zeta_a(1) + \frac{173}{9} \zeta_a(3) - \frac{110}{9} \zeta_a(5) - \frac{110}{9} \zeta_a(1) \cdot \zeta_a(3) + \frac{170}{9} \zeta_a(1) \cdot \zeta_a(5) - \frac{17}{3} \zeta_a^2(3)\}, \\
P(5) &= \frac{1}{6} \{1 - 20\zeta_a(1) + \frac{281}{3} \zeta_a(3) - \frac{1355}{6} \zeta_a(5) + \frac{889}{6} \zeta_a(7) - 180\zeta_a(1) \cdot \zeta_a(3) + \frac{3920}{3} \zeta_a(1) \cdot \zeta_a(5) - \frac{3290}{3} \zeta_a(1) \cdot \zeta_a(7) - \frac{170}{3} \zeta_a(3) \cdot \zeta_a(5) + 670\zeta_a(3) \cdot \zeta_a(7) - 326\zeta_a^2(3) - 970 \zeta_a^2(5)\}. \\
\end{align*}
$$

(1.16)

The values of the Riemann zeta function at odd arguments appear in several places in theoretical physics, not to mention in pure mathematics. Transcendental number $\zeta(3)$ first appeared in the expression for correlation functions in Takahashi’s papers [13, 24]. He evaluated the second neighbor correlation

$$\langle \mathbf{S}_i \cdot \mathbf{S}_{i+2} \rangle = \frac{1}{4} = 4 \ln 2 + \frac{9}{4} \zeta(3)$$  \hspace{1cm} (1.17)

It was obtained from the $1/U$ expansion of the ground state energy for the half-filled Hubbard chain (see also another derivation in ref. [23]). We remark that the expression for $P(3)$ (1.7) can be extracted from (1.17).

Now let us discuss the asymptotic behavior of $P(n)$ when $n$ is large. At zero temperature we believe that $P(n)$ should show a Gaussian decay as $n$ tends to infinity [14, 15]. In order to prove it mathematically we have to obtain a general formula for $P(n)$ which has not been achieved yet. On the other hand, we can calculate $P(n)$ by numerical means and confirm our analytical results. We have applied the Density Matrix Renormalization Group (DMRG) method [23, 22, 24] and obtained more numerical values of $P(n)$. The result is given in the end of section 2. At finite temperature it was shown that $P(n)$ decays exponentially [10]. This time we can employ the Quantum Monte-Carlo (QMC) simulation [23] to calculate $P(n)$ numerically. In section 3 we confirm that $P(n)$ exhibits an exponential decay at finite temperature and confirm our analytical expression. Let us note that this numerical approach was successfully applied to the XX model in ref. [12].

2 $P(n)$ at zero temperature

The integral representation of $P(n)$ for the XXX chain was obtained in [8] based on the vertex operator approach [8]

$$
P(n) = \int_{\mathcal{C}} \frac{d\lambda_1}{2\pi i \lambda_1} \int_{\mathcal{C}} \frac{d\lambda_2}{2\pi i \lambda_2} \cdots \int_{\mathcal{C}} \frac{d\lambda_n}{2\pi i \lambda_n} \prod_{a=1}^{n} (1 + \frac{i}{\lambda_a}) n-a \left(\frac{\pi \lambda_a}{\sinh \pi \lambda_a}\right)^n \prod_{1 \leq j < k \leq n} \sinh \pi (\lambda_k - \lambda_j - i). \hspace{1cm} (2.1)
$$
The contour $C$ in each integral goes parallel to the real axis with the imaginary part between 0 and $-i$. Below we sketch the evaluation of the integral for $P(5)$. It can be written in the following form

$$P(5) = \prod_{j=1}^{5} \int_{C} \frac{d\lambda_{j}}{2\pi i} U_{5}(\lambda_{1}, \ldots, \lambda_{5}) T_{5}(\lambda_{1}, \ldots, \lambda_{5}),$$

where

$$U_{5}(\lambda_{1}, \ldots, \lambda_{5}) = \pi^{15} \prod_{1 \leq k < j \leq 5} \sinh \pi(\lambda_{j} - \lambda_{k}) \prod_{j=1}^{5} \sinh \pi \lambda_{j},$$

and

$$T_{5}(\lambda_{1}, \ldots, \lambda_{5}) = \prod_{1 \leq k < j \leq 5} (\lambda_{j} + i)^{5-j} \prod_{j=1}^{5} (\lambda_{j} - \lambda_{k} - i).$$

Taking into account the properties of the functions $U_{5}(\lambda_{1}, \ldots, \lambda_{5})$, one can reduce the integrand $T_{5}(\lambda_{1}, \ldots, \lambda_{5})$ to the “canonical form”, $T_{5}^{2}(\lambda_{1}, \ldots, \lambda_{5})$ as was done for $P(2)$, $P(3)$ and $P(4)$ in ref. [1]

$$T_{5}^{2}(\lambda_{1}, \ldots, \lambda_{5}) = P_{0}^{(5)} + \frac{P_{1}^{(5)}}{\lambda_{2} - \lambda_{1}} + \frac{P_{2}^{(5)}}{(\lambda_{2} - \lambda_{1})(\lambda_{4} - \lambda_{3})},$$

where the $P^{(0)}$, $P^{(1)}$, $P^{(2)}$ are polynomials of the integration variables $\lambda_{1}, \ldots, \lambda_{5}$. The manifest form of these polynomials is shown in Appendix.

Now using the methods developed in [1] we can calculate three integrals that contribute into $P(5)$

$$J_{0}^{(5)} = \prod_{j=1}^{5} \int_{C} \frac{d\lambda_{j}}{2\pi i} U_{5}(\lambda_{1}, \ldots, \lambda_{5}) P_{0}^{(5)}(\lambda_{1}, \ldots, \lambda_{5}),$$

$$J_{1}^{(5)} = \prod_{j=1}^{5} \int_{C} \frac{d\lambda_{j}}{2\pi i} U_{5}(\lambda_{1}, \ldots, \lambda_{5}) \frac{P_{1}^{(5)}(\lambda_{1}, \ldots, \lambda_{5})}{\lambda_{2} - \lambda_{1}},$$

$$J_{2}^{(5)} = \prod_{j=1}^{5} \int_{C} \frac{d\lambda_{j}}{2\pi i} U_{5}(\lambda_{1}, \ldots, \lambda_{5}) \frac{P_{2}^{(5)}(\lambda_{1}, \ldots, \lambda_{5})}{(\lambda_{2} - \lambda_{1})(\lambda_{4} - \lambda_{3})}.$$

The result looks as follows:

$$J_{0}^{(5)} = \frac{689}{576} \tag{2.9}$$

$$J_{1}^{(5)} = \frac{-593}{576} - \frac{10}{3} \ln 2 - \frac{2773}{384} \zeta(3) - \frac{175}{48} \zeta(5) + \frac{13727}{1024} \zeta(7), \tag{2.10}$$

$$J_{2}^{(5)} = \frac{2423}{128} \zeta(3) - \frac{45}{2} \ln 2 \cdot \zeta(3) - \frac{489}{16} \zeta(3)^{2} - \frac{2025}{64} \zeta(5) + \frac{1225}{6} \ln 2 \cdot \zeta(5) - \frac{425}{64} \zeta(3) \cdot \zeta(5) - \frac{12125}{512} \zeta(7)^{2} + \frac{11165}{1024} \zeta(7) - \frac{11515}{64} \ln 2 \cdot \zeta(7) + \frac{42777}{512} \zeta(3) \cdot \zeta(7). \tag{2.11}$$

Summing up these three values we come to our final answer \[ \boxed{[13].} \]

Using the same method we can, in principle, get the analytic formula for any $P(n)$. Unfortunately, so far we have not succeeded in calculating $P(n)$ for $n \geq 6$. On the other hand, one can estimate the numerical values of $P(n)$ using DMRG [24, 23]. The method is suitable for studying ground-state properties. We followed standard algorithm, which can be found in literature (see ref. [24]). Below we shall outline some technical points that are relevant for the simulation precision. We implemented the infinite-system method. We have repeated renormalization 200-times. At each renormalization, we kept, at most, 200 relevant states for a (new) block; namely, we set $m = 200$. The density-matrix eigenvalue \{w_{n}\} of remaining bases indicates the statistical weight. We found $w_{n} > 10^{-10}$: That is, we have remained almost all relevant states with appreciable statistical weight $w_{n} > 10^{-10}$ through numerical renormalizations. In other words, we have discarded (disregarded) those states with exceedingly small statistical weight $w_{n} < 10^{-10}$, which may indicate error of the present simulation.

The obtained data are shown in Table \[ \boxed{[1].} \] Compared with the exact values \[ \boxed{[1], [2], [3], [4].} \] we see the DMRG data achieve about 3 digits accuracy up to $P(5)$. Probably the other data, i.e., $P(6), \ldots, P(8)$ also maintain at least 1 or 2 digits accuracy. Then combining the exact values up to $P(5)$ and the numerical data in Table 1, we have made a semi-log plot in Fig. 1. On the vertical axis we plotted the $\ln P(n)$, on horizontal axis we plotted $n^{2}$. From Fig.1 we clearly see the data fall into a straight line suggesting that the asymptotic form of $P(n)$ is governed by the Gaussian form,

$$P(n) \sim a^{-n^{2}}. \tag{2.12}$$
Table 1: DMRG data for $P(n)$ with uncertainties in the final digits.

| $n$ | $P(n)$ by DMRG |
|-----|----------------|
| 2   | $1.0222 \times 10^{-1}$ |
| 3   | $7.6238 \times 10^{-3}$ |
| 4   | $2.0607 \times 10^{-4}$ |
| 5   | $2.011 \times 10^{-6}$ |
| 6   | $7.05 \times 10^{-9}$ |
| 7   | $8.85 \times 10^{-12}$ |
| 8   | $3.7 \times 10^{-15}$ |

We can read off the Gaussian decay rate $a$ from the slope. Our estimate is $a = 1.6719 \pm 0.0005$. It is an intriguing open problem to associate this number with a certain analytical expression. Doctor A.G. Abanov confirmed Gaussian form of asymptotic expression in the frame of bosonization technique.

![Figure 1: $P(n)$ at zero temperature](image)

3 $P(n)$ at finite temperature by QMC simulation

At finite temperature $T$ the emptiness formation probability $P(n)$ is defined by the thermal average

$$P(n) = \frac{\text{Tr} \left\{ e^{-H/T} \prod_{j=1}^{n} P_j \right\}}{\text{Tr} \left\{ e^{-H/T} \right\}}. \quad (3.1)$$

It was shown in ref. [10] that $P(n)$ decays exponentially at finite temperature as $n$ goes to infinity

$$P(n) \sim c_0(T) e^{-nf}.$$ \quad (3.2)

Here $f$ is the free energy per site of the system and $c_0(T)$ is a constant prefactor. We shall confirm this formula by calculating $P(n)$ numerically by QMC simulation [24]. We adopted the continuous-time algorithm [24] with the cluster-flip update [27, 28, 29] which is completely free from the Trotter-decomposition error. We treated system sizes up to $N = 128$, and imposed the periodic boundary condition. We performed five-million Monte-Carlo steps initiated by 0.5 million steps for reaching thermal equilibrium. $P(n)$ is measured over the five-million Monte-Carlo steps. The semi-log plots of the data for several different temperatures are shown in Fig. 2. The straight lines (slopes) are the analytic asymptotic formula (3.2). We assumed $c_0(T) = 1$ for simplicity. Actually $c_0(T)$ deviates from unity for low temperature. Anyway we observe that as $n \to \infty$, EFP $P(n)$ decays exponentially according to the asymptotic form (3.2). In particular, at sufficiently high temperatures, even for small $n$, EFP $P(n)$ is well fitted by (3.2). In contrast, at low temperature, when $n$ becomes small $P(n)$ may reflect the Gaussian decay at zero temperature and deviates from (3.2). It agrees with the physical picture. Since, zero temperature is a critical point, we expect qualitative change of asymptotic of correlation functions.

Finally let us make a comment how we can evaluate the free energy per site $f$ from the point of view of the Bethe Ansatz. There are now three different integral equations which determine the free energy $f$.
1. Thermodynamic Bethe Ansatz (TBA) equations formulated by Takahashi [30] based on the string hypothesis.

2. Non-linear Integral Equations (NLIE) found by Klümper [31, 32] and Destri–de Vega [33] in the development of the quantum transfer matrix method [34, 35, 36, 37].

3. New integral equation derived by Takahashi [38]. The third one was recently discovered in an attempt to simplify the TBA equations [38]. It has also a close connection with the quantum transfer matrix [39]. The equation is explicitly given by

\[
u(x) = 2 + \oint_C \left( \frac{1}{x - y - 2i} \exp \left[ \frac{2J/T}{(y + i)^2 + 1} \right] + \frac{1}{x - y + 2i} \exp \left[ \frac{2J/T}{(y - i)^2 + 1} \right] \right) \frac{1}{u(y)} \frac{dy}{2\pi i},
\]

where the contour \(C\) is a loop which counterclockwise encircles the origin. Numerically these three approaches provide perfectly the same data for free energy per site \(f\).

![Figure 2: \(P(n)\) at finite temperature](image)

**4 Conclusion**

Let us mention again that the main result of this paper is the calculation of \(P(5)\) by means of the multi-integral representation. It is expressed only in terms of \(\ln 2\) and Riemann zeta function with odd arguments with rational coefficients. This should be the general property of \(P(n)\). We expect that other correlation functions such as \(\langle S_j S_k \rangle\) will share this property.

We have calculated numerically the value of \(P(n)\) and considered the asymptotic behavior. As was discussed in ref. [10], EFP \(P(n)\) shows a Gaussian decay at zero temperature, while it decays exponentially at finite temperature.

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**A Appendix**

Here we show the polynomials \(P_0^{(5)}, P_1^{(5)}, P_2^{(5)}\) which participate in the “canonical form” \(T_5^c\) given by the formula [23].

\[
P_0^{(5)} = \frac{689}{18} \lambda_2 \lambda_3^2 \lambda_4 \lambda_5^4
\]  

(A.1)
\[ P_1^{(5)} = \begin{pmatrix} 79633 & 3299 & 13844 & 16517 & 13463 \\ 15120 & 63 & 315 & 105 & 1512 \\ 1217491 & 840 & 279917 & 630 & 543079 \\ 14 & 126 & 7560 & 1260 & 36 \\ 9635 & 36199 & 811901 & 392107 & 12503 \\ 8 & 126 & 7560 & 1260 & 36 \\ 66721 & 6301 & 50921 & 7560 & 1260 \\ 1512 & 126 & 7560 & 1260 & 36 \\ 19549 & 7560 & 1260 & 36 \\ 87209 & 5041 & 1260 & 36 \\ 42262 & 189 & 126 & 36 \\ 189 & 126 & 36 \\ \end{pmatrix} \]

\[ P_2^{(5)} = \begin{pmatrix} 40111 & 202861 & 3523 & 6121 & 3433 \\ 15120 & 36 & 126 & 9 & 36 \\ 4813 & 1309 & 40 & 9 & 40 \\ 9 & 1890 & 126 & 9 & 126 \\ 582137 & 76147 & 1640 & 350 & 16229 \\ 5040 & 120 & 36 & 9 & 36 \\ \end{pmatrix} \]

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