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Quantum spin chains and Riemann zeta function with odd arguments

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Abstract
The Riemann zeta function is an important object of number theory. We argue that it is related to the Heisenberg spin-$1/2$ anti-ferromagnet. In the *XXX* spin chain we study the probability of formation of a ferromagnetic string in the anti-ferromagnetic ground state in the thermodynamics limit. We prove that for short strings the probability can be expressed in terms of the Riemann zeta function with odd arguments.

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1. Introduction

The Riemann zeta function for $\mathrm{Re}\,(s) > 1$ can be defined as follows:

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}. \tag{1.1}$$

It also can be represented as a product with respect to all prime numbers p

$$\zeta(s) = \prod_p (1 - p^{-s})^{-1}. \tag{1.2}$$

It can be analytically continued in the whole complex plane of s. It has only one pole, at $s = 1$, and it has 'trivial' zeros at $s = -2n$ ($n > 1$ is an integer). The famous Riemann hypothesis [1] states that nontrivial zeros belong to the straight line $\mathrm{Re}\,(s) = 1/2$. The Riemann zeta function is useful for the study of distribution of prime numbers on the real axis [2]. At even values of its argument the zeta function can be expressed in terms of powers of π. Mathematicians believe that at odd values of its argument $\zeta(n)$ is an irrational number (this was proven for $\zeta(3)$). The Riemann zeta function also appears in theoretical physics. Some Feynman diagrams in quantum field theory can be expressed in terms of $\zeta(n)$ (see, e.g., [3]). It also appears in string theory [4].

We argue that $\zeta(n)$ is also important for exactly solvable models. The most famous integrable model is the Heisenberg *XXX* spin chain. This model was first suggested by Heisenberg [5] in 1928 and solved by Bethe [6] in 1931. Since that time it has found multiple applications in solid state physics and statistical mechanics. Recently the *XXX* spin chain was used for study of the entanglement in quantum computations [7].

The Hamiltonian of the *XXX* spin chain can be written as follows:

$$H = \sum_{i=1}^{N} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \sigma_i^z \sigma_{i+1}^z - 1). \tag{1.3}$$

Here N is the length of the lattice and $\sigma_i^x, \sigma_i^y, \sigma_i^z$ are Pauli matrices. We consider the thermodynamics limit, when $N -> \infty$. The sign in front of the Hamiltonian indicates that we are considering the anti-ferromagnetic case. We consider periodic boundary conditions. Notice that this Hamiltonian annihilates the ferromagnetic state (all spins up).

The construction of the anti-ferromagnetic ground state wavefunction $|\mathrm{AFM}\rangle$ can be credited to Hulthén [8]. An important correlation function was defined in [9]. It was called the emptiness formation probability

$$P(n) = \langle \mathrm{AFM}| \prod_{j=1}^{n} P_j |\mathrm{AFM}\rangle$$

where $P_j = (1+\sigma_j^z)/2$ is a projector on the state with spin up in the jth lattice site. Averaging is over the anti-ferromagnetic ground state. It describes the probability of formation of a ferromagnetic string of length n in the anti-ferromagnetic background $|\mathrm{AFM}\rangle$. In this paper we shall first study short strings (n is small); at the end we shall discuss long-distance asymptotics (at finite temperature). The four first values of the emptiness-formation probability appear as follows:

$$P(1) = \tfrac{1}{2} = 0.5 \tag{1.4}$$

$$P(2) = \tfrac{1}{3} - \tfrac{1}{3}\ln 2 = 0.102\,284\,273 \tag{1.5}$$

$$P(3) = \tfrac{1}{4} - \ln 2 + \tfrac{3}{8}\zeta(3) = 0.007\,624\,158 \tag{1.6}$$

$$\begin{aligned} P(4) = {} & \tfrac{1}{5} - 2\ln 2 + \tfrac{173}{60}\zeta(3) - \tfrac{11}{6}\zeta(3)\ln 2 - \tfrac{51}{80}\zeta^2(3) \\ & - \tfrac{55}{24}\zeta(5) + \tfrac{85}{24}\zeta(5)\ln 2 = 0.000\,206\,270. \end{aligned} \tag{1.7}$$

Let us comment. The value of $P(1)$ is evident from the symmetry; $P(2)$ can be extracted from the explicit expression of the ground state energy [8]. $P(3)$ can be extracted from the results of Takahashi [10] on the calculation of the nearest-neighbour correlation. This was confirmed in [11]. One should also mention the independent calculation of $P(3)$ in [12]. One can express $P(3)$ in terms of next-nearest-neighbour correlation

$$\langle S_i^z S_{i+2}^z \rangle = 2\,P(3) - 2\,P(2) + \tfrac{1}{2}\,P(1). \tag{1.8}$$

The calculation of $P(3)$ and $P(4)$ is discussed in this paper.

The expression above for $P(4)$ is our main result here.

The plan of the paper is as follows. In the next section we discuss some main steps of the calculation of $P(3)$ and $P(4)$. The thermodynamics of $P(n)$ for non-zero temperature is briefly discussed in section 3. Then we summarize the results in the conclusion.

2. General discussion of the calculation of $P(3)$ and $P(4)$

There are several different approaches to investigate $P(n)$:

- representation of correlation functions as determinants of Fredholm integral operators described in detail in the book [13] and
- the vertex operator approach developed by the RIMS group [14].

One can also mention the application of connection with other correlation functions, for instance, the correlation function $\langle \mathrm{AFM}|S_i^z S_{i+n}^z|\mathrm{AFM}\rangle$.

We shall use the integral representation obtained by Korepin *et al* [9] in the framework of the vertex operator approach at zero magnetic field:

$$P(n) = \int_C \frac{\mathrm{d}\lambda_1}{2\pi \mathrm{i}\lambda_1} \int_C \frac{\mathrm{d}\lambda_2}{2\pi \mathrm{i}\lambda_2} \cdots \int_C \frac{\mathrm{d}\lambda_n}{2\pi \mathrm{i}\lambda_n} \prod_{a=1}^{n} \left(1 + \frac{\mathrm{i}}{\lambda_a}\right)^{n-a} \left(\frac{\pi\lambda_a}{\sinh \pi\lambda_a}\right)^n \times \prod_{1\leqslant k<j\leqslant n} \frac{\sinh \pi(\lambda_j - \lambda_k)}{\pi(\lambda_j - \lambda_k - i)}. \tag{2.1}$$

The contour C in each integral goes parallel to the real axis with the imaginary part between zero and $-\mathrm{i}$.

Recently such a formula was generalized by de Gier and Korepin in [15] to the case where averaging is done over an arbitrary Bethe state (with no strings) instead of the antiferromagnetic state.

Let us describe in general the strategy we used in order to arrive at the answers (1.6) and (1.7). The integral formula (2.1) can be easily represented as follows:

$$P(n) = \pi^{\frac{n(n+1)}{2}} \prod_{j=1}^{n} \int_C \frac{\mathrm{d}\lambda_j}{2\pi \mathrm{i}}\, U(\lambda_1, \ldots, \lambda_n)\, T(\lambda_1, \ldots, \lambda_n) \tag{2.2}$$

where

$$U(\lambda_1, \ldots, \lambda_n) = \frac{\prod_{1\leqslant k<j\leqslant n} \sinh \pi(\lambda_j - \lambda_k)}{\prod_{j=1}^{n} \sinh^n \pi\lambda_j} \tag{2.3}$$

and

$$T(\lambda_1, \ldots, \lambda_n) = \frac{\prod_{j=1}^{n} \lambda_j^{j-1} (\lambda_j + \mathrm{i})^{n-j}}{\prod_{1\leqslant k<j\leqslant n} (\lambda_j - \lambda_k - \mathrm{i})}. \tag{2.4}$$

As is apparent we can make many simplifications without taking integrals but using some simple observations. First of all, let us note that the function $U(\lambda_1, \ldots, \lambda_n)$ is antisymmetric with respect to transposition of any pair of integration variables, say λ_j and λ_k. This simple observation turns out to be very useful because

$$\prod_{j=1}^{n} \int_C \frac{\mathrm{d}\lambda_j}{2\pi \mathrm{i}}\, U(\lambda_1, \ldots, \lambda_n)\, S(\lambda_1, \ldots, \lambda_n) = 0 \tag{2.5}$$

if the function S is symmetric for at least one pair of λ.

The next observation is also trivial; namely, we can try to reduce the power of the denominator in (2.4) using simple algebraic relations such as

$$\frac{1}{x(x+a)} = \frac{1}{ax} - \frac{1}{a(x+a)}. \tag{2.6}$$

Combining these two simple observations one can reduce integration functions for $P(3)$ to a sum of terms with denominators of power two and for $P(4)$ to a more complicated sum of terms with denominators of power not higher than three.

In order to calculate the integrals one can close the contours in the complex plane by the infinite semi-circles either in the upper half-plane or in the lower half-plane, not changing the integrals. Then it is possible to apply the Cauchy theorem using the following formulae:

$$\oint_{C_l} \mathrm{d}z \, \frac{f(z)}{\sinh^3 \pi z} = -\frac{(-1)^l}{2\pi} \left(1 - \frac{1}{\pi^2} \frac{\partial^2}{\partial \epsilon^2}\right)_{\epsilon \to 0} f(\mathrm{i}\, l + \epsilon) \tag{2.7}$$

$$\oint_{C_l} \mathrm{d}z \, \frac{f(z)}{\sinh^4 \pi z} = -\frac{2}{3\pi^2} \left(\frac{\partial}{\partial \epsilon} - \frac{1}{4\pi^2} \frac{\partial^3}{\partial \epsilon^3}\right)_{\epsilon \to 0} f(\mathrm{i}\, l + \epsilon) \tag{2.8}$$

for the cases $n = 3$ and 4 respectively where C_l is a small contour surrounding the point $\mathrm{i}\, l$ with an integer l in the anti-clockwise direction.

Then the integrals can be expressed in terms of the differential operator acting on some functions. For instance, for the case $n = 3$

$$\int_C \frac{\mathrm{d}\lambda_1}{2\pi \mathrm{i}} \int_C \frac{\mathrm{d}\lambda_2}{2\pi \mathrm{i}} \int_C \frac{\mathrm{d}\lambda_3}{2\pi \mathrm{i}} U(\lambda_1, \lambda_2, \lambda_3) F(\lambda_1, \lambda_2, \lambda_3) = \mathrm{D}\, \tilde{F}(\epsilon_1, \epsilon_2, \epsilon_3) \tag{2.9}$$

where D is the differential operator

$$\begin{aligned} \mathrm{D} = -\frac{\pi^3}{8} &\left(1 - \frac{1}{\pi^2} \frac{\partial^2}{\partial {\epsilon_1}^2}\right) \left(1 - \frac{1}{\pi^2} \frac{\partial^2}{\partial {\epsilon_2}^2}\right) \left(1 - \frac{1}{\pi^2} \frac{\partial^2}{\partial {\epsilon_3}^2}\right)_{\epsilon_1, \epsilon_2, \epsilon_3 \to 0} \\ &\times \sinh \pi(\epsilon_2 - \epsilon_1) \, \sinh \pi(\epsilon_3 - \epsilon_1) \, \sinh \pi(\epsilon_3 - \epsilon_2) \end{aligned} \tag{2.10}$$

and

$$\tilde{F}(\epsilon_1, \epsilon_2, \epsilon_3) = \sum_{l_1=0}^{\infty} (-1)^{l_1} \sum_{l_2=0}^{\infty} (-1)^{l_2} \sum_{l_3=0}^{\infty} (-1)^{l_3} F(\mathrm{i}\, l_1 + \epsilon_1, \mathrm{i}\, l_2 + \epsilon_2, \mathrm{i}\, l_3 + \epsilon_3). \tag{2.11}$$

Here all three contours were closed in the upper half-plane but in real calculations it turns out to be more convenient to close some of them in the lower half-plane, taking into consideration the appearance of an additional sign.

It is not difficult to obtain generalization of these formulae to the case $n = 4$, so the problem is reduced to the calculation of sums such as (2.11), expanding the result into the series in powers of ϵ and applying the differential operator D. This procedure is straightforward but can be rather tedious especially for the case $n = 4$. Proceeding in this way we can arrive at the results (1.6) and (1.7).

Let us note that both of these final answers appear to be expressed in terms of the logarithmic function and the Riemann zeta function of odd arguments and do not depend on polylogarithms in spite of the fact that polylogarithm $\mathrm{Li}_4(1/2)$ appears in the intermediate stage of calculation. All coefficients before these functions in (1.4)–(1.7) are rational. Moreover, they do not contain any powers of π which could be considered as Riemann zeta functions of even arguments.

Our conjecture is that the final answer for any $P(n)$ will also be expressed in terms of logarithm $\ln 2$ and Riemann zeta functions $\zeta(k)$ with odd integers k and with rational coefficients.

3. Thermodynamics of $P(n)$

If we had the exact answer for $P(n)$ for any n we could calculate an asymptotic of $P(n)$ when n tends to infinity. Unfortunately, at the moment we cannot do this because we have $P(n)$ only for $n = 1, 2, 3, 4$. Nevertheless we can discuss a possible behaviour of $P(n)$ with $n \to \infty$ using some other arguments.

For non-zero temperature one can conclude that the asymptotic of the partition function in the thermodynamic limit is as follows:

$$Z = \langle \mathrm{e}^{\frac{H}{kT}} \rangle \sim \mathrm{e}^{\frac{Nf}{kT}} \tag{3.1}$$

where f is the free energy per site and N is the length of the chain; it was evaluated in [16–18]. In fact, for $P(n)$ the n neighbouring spins are frozen. Therefore one has the asymptotics of $P(n)$ when n tends to infinity:

$$P(n) = \frac{\left\langle \prod_{j=1}^{n} \frac{(1+\sigma_j^z)}{2} \mathrm{e}^{\frac{H}{kT}} \right\rangle}{Z} \sim \frac{\mathrm{e}^{\frac{(N-n)f}{kT}}}{Z} = \mathrm{e}^{-\frac{nf}{kT}}. \tag{3.2}$$

For zero temperature we expect Gaussian decay.

4. Conclusion

Let us repeat that the main result of this paper is the calculation of $P(3)$ and $P(4)$ (1.6), (1.7) by means of the multi-integral representation (2.1). The fact that only the logarithm ln 2 and Riemann zeta function with odd arguments participate in the answers for $P(1), \ldots, P(4)$ and with rational coefficients before these functions allows us to suppose that this is the general property of $P(n)$. One could compare the calculation of $P(n)$ with the many-loop calculation of the self-energy diagrams in the renormalizable quantum field theory, which can also be expressed in terms of ζ functions of odd arguments [3].

Unfortunately, so far we do not have even a conjecture for $P(n)$, but we believe that this is not an unsolvable problem. Maybe already after calculation of $P(5)$ one could guess the right formula for a generic case $P(n)$. This would give an answer to the question discussed in the previous section, namely, the question about the law of decay of $P(n)$ when n tends to infinity.

Also it would be interesting to generalize the above results to the *XXZ* spin chain. Some interesting conjectures were recently proposed by Razumov and Stroganov [19] for the special case of the *XXZ* model with $\Delta = -1/2$. These conjectures would be supported if it were possible to obtain $P(n)$ from the general integral representation obtained by the RIMS group [14].

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