Quantum Spin Chains and Riemann Zeta Function with Odd Arguments

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Abstract

Riemann zeta function is an important object of number theory. We argue that it is related to 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. We prove that for short strings the probability can be expressed in terms of Riemann zeta function with odd arguments.

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1. Introduction

Riemann zeta function for $Re(s) > 1$ 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 [18] states that nontrivial zeros belong to the straight line $Re(s) = 1/2$. Riemann zeta function is useful for study of distribution of prime numbers on the real axis [17]. Mathematicians believe that at odd values of its argument $\zeta(n)$ is an irrational number [this was proven for $\zeta(3)$]. Riemann zeta function also appears in theoretical physics. Some Feynman diagrams in quantum field theory can be expressed in terms of $\zeta(n)$, see, for example, [1] . It appears also in string theory [2].

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 [3] in 1928 and solved by Bethe [4] in 1931 . Since that time it 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 [6].

The Hamiltonian of the XXX spin chain can be written like this

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

Here N is the length of the lattice and $\sigma_i^x, \sigma_i^y, \sigma_i^z$ are Pauli matrices. 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 wave function $|AFM>$ can be credited to Hulthén [5]. An important correlation function was defined in [12]. It was called the emptiness formation probability

$$P(n) =< AFM| \prod_{j=1}^{n} P_j |AFM >$$

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

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

$$P(2) \;=\; \frac{1}{3}(1 \;-\; \ln 2) \;=\; 0.102284273, \tag{1.5}$$

$$P(3) \;=\; \frac{1}{4} \;-\; \ln 2 \;+\; \frac{3}{8}\,\zeta(3) \;=\; 0.007624158, \tag{1.6}$$

$$\begin{aligned} P(4) \;=\; & \frac{1}{5} \;-\; 2\ln 2 \;+\; \frac{173}{60}\zeta(3) \;-\; \frac{11}{6}\zeta(3)\,\ln 2 \;-\; \frac{51}{80}\zeta^2(3) \\ & -\; \frac{55}{24}\zeta(5) \;+\; \frac{85}{24}\zeta(5)\,\ln 2 \;=\; 0.000206270 \end{aligned} \tag{1.7}$$

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 [5]. $P(3)$ can be extracted from the results of M.Takahashi [13]. One should also mention independent calculation of $P(3)$ in [14]. One can express $P(3)$ in terms of next to the nearest neighbor correlation

$$<\; S^z_i S^z_{i+2} \;> = \; 2\,P(3) \;-\; 2\,P(2) \;+\; \frac{1}{2}\,P(1) \tag{1.8}$$

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 the 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 [10]
- **the vertex operator approach** developed by the RIMS group [11]

One can also mention the application of connection with other correlation functions, for instance, the correlation function $< AFM|S^z_i S^z_{i+n}|AFM >$.

We shall use the integral representation obtained by Korepin, Izergin, Essler and Uglov [12] in framework of the vertex operator approach at the zero magnetic field:

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

The contour C in each integral goes parallel to the real axis with the imaginary part between 0 and $-i$.

Recently such formula was generalized by de Gier and Korepin in paper [15] to the case, where averaging is done over arbitrary Bethe state [with no strings] instead of anti-ferromagnetic state.

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

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

where

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

and

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

As appeared we can make a lot of 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 in 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

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

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

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

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

Combining these two simple observations one can reduce integration functions for $P(3)$ to a sum of terms with denominators of power 2 and for $P(4)$ to a more complicated sum of terms with denominators of power not higher than 3.

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

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

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

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

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

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

where D is the differential operator

$$D \;=\; \frac{\pi^3}{8i}\,(1-\frac{1}{\pi^2}\frac{\partial^2}{\partial{\epsilon_1}^2})(1-\frac{1}{\pi^2}\frac{\partial^2}{\partial{\epsilon_2}^2})(1-\frac{1}{\pi^2}\frac{\partial^2}{\partial{\epsilon_3}^2})_{\epsilon_1,\epsilon_2,\epsilon_3\to 0}$$

$$\sinh\pi(\epsilon_2-\epsilon_1)\,\sinh\pi(\epsilon_3-\epsilon_1)\,\sinh\pi(\epsilon_3-\epsilon_2) \tag{2.10}$$

and

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

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 another direction taking into consideration appearance of an additional sign.

It is not difficult to get generalization of these formulae to the case $n = 4$. So the problem is reduced to the calculation of sums like (2.11), expanding the result into the series in powers of ϵ-s 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 come to the results (1.6) and (1.7).

Let us note that both of these final answers appeared 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 $\mathrm{Li}_4(1/2)$ appeared in the intermediate stage of calculation. All coefficients before those functions in (1.4-1.7) are rational. Also 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 asymptotics of $P(n)$ when n tends to infinity. Unfortunately, for a moment we can not do this because we have $P(n)$ only for $n = 1, 2, 3, 4$. Nevertheless we can discuss a possible behavior of $P(n)$ with $n \to \infty$ using some other arguments.

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

$$Z \;=<\; e^{\frac{H}{kT}} \;>\sim\; e^{\frac{Nf}{kT}} \tag{3.1}$$

where f is the free energy per site and N is the length of the chain, it was evaluated in [7], [8] and [9]. In fact, for $P(n)$ the n neighboring spins are frozen. Therefore one has the asymptotics of $P(n)$ when n tends to infinity

$$P(n) \;=\; \frac{<\,\prod_{j=1}^{n}\frac{(1+\sigma_j^z)}{2}\;e^{\frac{H}{kT}}\;>}{Z} \;\sim\; \frac{e^{\frac{(N-n)f}{kT}}}{Z} \;=\; e^{-\frac{nf}{kT}} \tag{3.2}$$

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 [1] .

Unfortunately, so far we have not got even a conjecture for $P(n)$ but we believe that it is not an unsolvable problem. May be already after calculation of $P(5)$ one could guess the right formula for a generic case $P(n)$. It 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 above results to the XXZ spin chain. Some interesting conjectures were recently invented by Razumov and Stroganov [16] for the special case of the XXZ model with $\Delta = -1/2$. These conjectures would be supported if it were possible to get $P(n)$ from the general integral representation obtained by the RIMS group [11].

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