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Spin chains and combinatorics: twisted boundary conditions

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Abstract

The finite XXZ Heisenberg spin chain with twisted boundary conditions is considered. For the case of an even number of sites N , anisotropy parameter $-1/2$ and twisting angle $2\pi/3$ the Hamiltonian of the system possesses an eigenvalue $-3N/2$. The explicit form of the corresponding eigenvector was found for $N \leq 12$. Conjecturing that this vector is the ground state of the system we made and verified several conjectures related to the norm of the ground state vector, its component with maximal absolute value and some correlation functions, which have combinatorial nature. In particular, we conjecture that the squared norm of the ground state vector coincides with the number of half-turn symmetric alternating sign $N \times N$ matrices.

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The Hamiltonian of the periodic XXZ Heisenberg spin chain with the number of sites N and the anisotropy parameter Δ has the form

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

where we assume that

$$\sigma_{N+1}^x = \sigma_1^x \quad \sigma_{N+1}^y = \sigma_1^y \quad \sigma_{N+1}^z = \sigma_1^z.$$

In terms of the operators $\sigma_i^+ = (\sigma_i^x + i \sigma_i^y)/2$, $\sigma_i^- = (\sigma_i^x - i \sigma_i^y)/2$ and σ_i^z one has the following expression for the Hamiltonian:

$$H^{(N)} = -2 \sum_{i=1}^N [\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+] - \Delta \sum_{i=1}^N \sigma_i^z \sigma_{i+1}^z \quad (1)$$

and the boundary conditions take the form

$$\sigma_{N+1}^+ = \sigma_1^+ \quad \sigma_{N+1}^- = \sigma_1^- \quad \sigma_{N+1}^z = \sigma_1^z. \quad (2)$$

It was proven in paper [1] that for $\Delta = -1/2$ and for an odd N the Hamiltonian $H^{(N)}$ has the eigenvalue $-3N/2$ (see also [2]). In our paper [3] we analysed the explicit expressions for the corresponding eigenvectors and made the conjecture, which was verified for $N \leq 17$, that the eigenvalue $-3N/2$ corresponds to the ground state of the system. This is in agreement with the earlier numerical results reported in paper [4]. In the same paper [3] we made and verified for $N \leq 17$ many conjectures concerning the norm of the ground state, the largest components of the ground state vector and some correlation functions. These conjectures have a combinatorial character and are related, in particular, to the number of alternating sign matrices (see, e.g., [5, 6]).

Several variations of the XXZ Heisenberg chain with a special ground state energy are also known [4, 7–9]. Very recently Batchelor, de Gier and Nienhuis considered these variations along with the corresponding $O(n)$ loop model at $n = 1$ [10]. They found the generalization for two of our conjectures for these systems and extended a list of related combinatorial objects.

First of all the authors of paper [10] reported on the XXZ Heisenberg chain with twisted boundary conditions. The Hamiltonian in this case has again form (1), but instead of (2) one uses the boundary conditions

$$\sigma_{N+1}^+ = e^{i\phi} \sigma_1^+ \quad \sigma_{N+1}^- = e^{-i\phi} \sigma_1^- \quad \sigma_{N+1}^z = \sigma_1^z.$$

Explicitly one can write

$$H^{(N)} = -2 \sum_{i=1}^{N-1} [\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+] - 2 e^{-i\phi} \sigma_N^+ \sigma_1^- - 2 e^{i\phi} \sigma_N^- \sigma_1^+ - \Delta \sum_{i=1}^N \sigma_i^z \sigma_{i+1}^z. \quad (3)$$

In [4] on the basis of numerical calculations it was conjectured that for the special value of the twisting angle $\phi = 2\pi/3$ and $\Delta = -1/2$ the ground state energy is equal to $-3N/2$. The proof of the existence of such an eigenvalue of the Hamiltonian was given in paper [9]. This was the case that was considered by the authors of paper [10]. They formulated two conjectures concerning the sum of the components of the supposed ground state vector and the sum of its squared components enjoying remarkable combinatorial character.

In the present paper we also consider the case $\phi = 2\pi/3$, $\Delta = -1/2$, and study the eigenvectors of the Hamiltonian (3) corresponding to the eigenvalue $-3N/2$ with the main purpose of finding conjectures on correlation functions. We start with exposition of the explicit form of the eigenvectors for $N = 2, 4, 6$. We hope that this information will help someone to further treat the problem. As a matter of fact we found explicitly the eigenvectors for $N = 8, 10$ and 12 as well, but they have 70, 252 and 924 components, respectively, so we decided against their exposition. Let us fix the notations.

We use the basis in the state space formed by the normed common eigenvectors of the operators σ_i^z . Here we associate \uparrow with the eigenvalue $+1$ and \downarrow with the eigenvalue -1 . Thus, the basis vectors are marked by words consisting of N letters \uparrow and \downarrow . The set of such words is denoted $W^{(N)}$ and we write for a general state vector

$$|\Psi\rangle = \sum_{A \in W^{(N)}} \Psi_A |A\rangle.$$

Furthermore, we use such representation for the operators σ_i^x and σ_i^y that their matrix elements coincide with usual Pauli matrices. Finally, the eigenvector of the Hamiltonian (3) with the eigenvalue $-3N/2$ is denoted $|\Psi^{(N)}\rangle$.

The eigenvector $|\Psi^{(2)}\rangle$ has the form

$$|\Psi^{(2)}\rangle = -\frac{i}{2} (1 + i\sqrt{3}) |\downarrow\uparrow\rangle + \frac{i}{2} (1 - i\sqrt{3}) |\uparrow\downarrow\rangle.$$

Let us discuss the used normalization condition. Consider the operator

$$R = \sigma_1^x \cdots \sigma_N^x$$

which reverses the z -action projection of the spins and the antiunitary operator K of complex conjugation acting on a general state vector as

$$K|\Psi\rangle = \sum_A \Psi_A^* |A\rangle.$$

It is clear that the Hamiltonian (3) commutes with the operator¹ $R' = RK$. Moreover, we have $R'^2 = 1$. We have found that for even $N \leq 12$ the eigenvalue $-3N/2$ is nondegenerate. It follows from these facts that multiplying $|\Psi^{(N)}\rangle$ by an appropriate phase factor one can satisfy the condition

$$R'|\Psi^{(N)}\rangle = |\Psi^{(N)}\rangle. \quad (4)$$

This condition is invariant under the multiplication of $|\Psi^{(N)}\rangle$ by a real number. To fix this freedom we divide $|\Psi^{(N)}\rangle$ by the least absolute value of its components. After this the vector $|\Psi^{(N)}\rangle$ is defined up to a sign which is fixed by the requirement that the sum of the components of $|\Psi^{(N)}\rangle$ be positive².

Under the above normalization conditions the vector $|\Psi^{(4)}\rangle$ looks like

$$\begin{aligned} |\Psi^{(4)}\rangle = & \frac{1}{2} (1 - i\sqrt{3}) |\downarrow\downarrow\uparrow\uparrow\rangle + \frac{1}{2} (3 - i\sqrt{3}) |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle \\ & + |\uparrow\downarrow\downarrow\uparrow\rangle + \frac{1}{2} (3 + i\sqrt{3}) |\uparrow\downarrow\uparrow\downarrow\rangle + \frac{1}{2} (1 + i\sqrt{3}) |\uparrow\uparrow\downarrow\downarrow\rangle. \end{aligned}$$

For the case $N = 6$ we obtain

$$\begin{aligned} |\Psi^{(6)}\rangle = & -i |\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle + \frac{1}{2} (\sqrt{3} - 5i) |\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle \\ & + (\sqrt{3} - 2i) |\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle + \frac{1}{2} (\sqrt{3} - i) |\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle + (\sqrt{3} - 2i) |\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle \\ & + \frac{5}{2} (\sqrt{3} - i) |\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle + \frac{1}{2} (3\sqrt{3} - i) |\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle + \frac{1}{2} (3\sqrt{3} - i) |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle \\ & + \frac{1}{2} (3\sqrt{3} + i) |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle + \frac{1}{2} (\sqrt{3} + i) |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle + \frac{1}{2} (\sqrt{3} - i) |\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle \\ & + \frac{1}{2} (3\sqrt{3} - i) |\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle + \frac{1}{2} (3\sqrt{3} + i) |\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle + \frac{1}{2} (3\sqrt{3} + i) |\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\rangle \\ & + \frac{5}{2} (\sqrt{3} + i) |\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\rangle + (\sqrt{3} + 2i) |\uparrow\downarrow\uparrow\downarrow\downarrow\uparrow\rangle + \frac{1}{2} (\sqrt{3} + i) |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\rangle \\ & + (\sqrt{3} + 2i) |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\rangle + \frac{1}{2} (\sqrt{3} + 5i) |\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\rangle + i |\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle. \end{aligned}$$

Actually Hamiltonian (3) has some shift invariance discussed below. This invariance reveals itself in the structure of the components of the vectors $|\Psi^{(N)}\rangle$. Due to the complex character of the components of the eigenvector $|\Psi^{(N)}\rangle$, our data are fewer than for the periodic case [3]. Nevertheless, we are able to formulate and verify analogues of conjectures given in [3]. The first conjecture associates the eigenvalue $-3N/2$ with the ground state.

Conjecture 1. The ground state of Hamiltonian (3) for an even N , $\phi = 2\pi/3$ and $\Delta = -1/2$ has the energy $E = -3N/2$ and the total spin z -axis projection $S_z = 0$.

Consider now the maximal and the minimal absolute value of the components of $|\Psi^{(N)}\rangle$. Note that the minimal absolute value is taken, in particular, by the ferromagnetic component $\Psi_{\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow}^{(N)}$ and the maximal absolute value is taken by the antiferromagnetic component $\Psi_{\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow}^{(N)}$. For the absolute value of the ratio $\Psi_{\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow}^{(2n)} / \Psi_{\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow}^{(2n)}$ we have the sequence

$$1, \quad \sqrt{3}, \quad 5, \quad 14\sqrt{3}, \quad 198, \quad 1573\sqrt{3}, \quad \dots \quad (5)$$

¹ The Hamiltonian (3) also commutes with the product of the operator reversing the direction of the chain and the operator K and such symmetry can be also used for the fixation of $|\Psi^{(N)}\rangle$.

² Note that this sum is real due to the condition (4).

Recall that for the periodic boundary conditions and an odd number of sites we have obtained [3] that the similar ratio $\Psi_{\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow}^{(2n+1)} / \Psi_{\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow}^{(2n+1)}$ coincides with the number A_n of the alternating sign $n \times n$ matrices. The numbers A_n are given by the formula

$$A_n = \prod_{i=0}^{n-1} \frac{(3i+1)!}{(n+i)!}$$

and the sequence A_n goes as

$$1, 2, 7, 42, 429, 7436, \dots \quad (6)$$

Dividing sequence (5) by sequence (6), we arrive at

$$1, \frac{\sqrt{3}}{2}, \frac{5}{7}, \frac{\sqrt{3}}{3}, \frac{6}{13}, \frac{11\sqrt{3}}{4 \cdot 13}, \dots \quad (7)$$

Let us now pay special attention to the largest prime divisors in the denominators, seven for $n = 3$ and 13 for $n = 5$. Their locations prompt us to consider the auxiliary sequence

$$1, 4, 4 \cdot 7, 4 \cdot 7 \cdot 10, 4 \cdot 7 \cdot 10 \cdot 13, 4 \cdot 7 \cdot 10 \cdot 13 \cdot 16, \dots \quad (8)$$

and to multiply sequence (7) by (8). This leads to

$$1, 2\sqrt{3}, 2^2 \cdot 5, \frac{2^3 \cdot 5 \cdot 7 \sqrt{3}}{3}, 2^4 \cdot 3 \cdot 5 \cdot 7, 2^5 \cdot 5 \cdot 7 \cdot 11\sqrt{3}, \dots \quad (9)$$

The largest prime divisors in the numerators hint at another auxiliary sequence

$$1, 3, 3 \cdot 5, 3 \cdot 5 \cdot 7, 3 \cdot 5 \cdot 7 \cdot 9, 3 \cdot 5 \cdot 7 \cdot 9 \cdot 11, \dots \quad (10)$$

Dividing sequence (9) by sequence (10), we arrive at

$$1, \frac{2}{\sqrt{3}}, \left(\frac{2}{\sqrt{3}}\right)^2, \left(\frac{2}{\sqrt{3}}\right)^3, \left(\frac{2}{\sqrt{3}}\right)^4, \left(\frac{2}{\sqrt{3}}\right)^5, \dots$$

As the result we obtain

Conjecture 2. The absolute value of the ratio of a component of $|\Psi^{(2n)}\rangle$ with the largest absolute value to the component with the smallest absolute value is given by the formula

$$\left| \frac{\Psi_{\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow}^{(2n)}}{\Psi_{\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow}^{(2n)}} \right| = \left(\frac{2}{\sqrt{3}}\right)^{n-1} \frac{1 \cdot 3 \cdot 5 \cdots (2n-3)(2n-1)}{1 \cdot 4 \cdot 7 \cdots (3n-5)(3n-2)} A_n.$$

Consider now the squared norm of the vector $|\Psi^{(N)}\rangle$:

$$\mathcal{N}_N^2 = \langle \Psi^{(N)} | \Psi^{(N)} \rangle = \sum_{A \in W^{(N)}} |\Psi_A^{(N)}|^2.$$

Fixing the normalization in the way discussed above we see that the sequence formed by the numbers \mathcal{N}_{2n}^2 goes as

$$2, 10, 140, 5544, 622\,908, 198\,846\,076, \dots \quad (11)$$

For the case of periodic boundary conditions the corresponding sequence of squared norms \mathcal{N}_{2n+1}^2 is

$$1, 3, 25, 588, 39\,204, 7422\,987, \dots \quad (12)$$

and we conjectured in [3] that

$$\mathcal{N}_{2n+1}^2 = \left(\frac{3}{4}\right)^n \left[\frac{2 \cdot 5 \cdots (3n-1)}{1 \cdot 3 \cdots (2n-1)} \right]^2 A_n^2.$$

Dividing sequence (11) by the sequence formed by the numbers A_n^2 , we obtain

$$2, \frac{5}{2}, \frac{2^2 \cdot 5}{7}, \frac{2 \cdot 11}{7}, \frac{2^2 \cdot 11}{13}, \frac{11 \cdot 17}{2^2 \cdot 13}, \dots$$

Using the same method as for conjecture 2, we arrive at the following analogue of conjecture 3 formulated in [3].

Conjecture 3. The squared norm of the vector $|\Psi^{(2n)}\rangle$ is given by the formula

$$\mathcal{N}_{2n}^2 = \frac{2 \cdot 5 \cdots (3n-1)}{1 \cdot 4 \cdots (3n-2)} A_n^2.$$

Let us remark that joining the sequences (11) and (12) we arrive at the sequence

1, 2, 3, 10, 25, 140, 588, 5544, 39 204, 622 908, 7422 987,

This is the sequence formed by the number of half-turn symmetric alternating sign $N \times N$ matrices A_N^{HT} (see [11, 12] and references therein). Therefore we can combine our conjecture 3 and conjecture 3 of [3] into the statement that $\mathcal{N}_N^2 = A_N^{\text{HT}}$.

Batchelor *et al* discovered another analogue of conjecture 3 of [3].

Conjecture 3' (Batchelor *et al* [10]). The sum of the squared components of the vector $|\Psi^{(2n)}\rangle$ is given by

$$\sum_{A \in W^{(2n)}} (\Psi_A^{(2n)})^2 = A_n^2.$$

The same authors gave the analogue of conjecture 4 from [3].

Conjecture 4 (Batchelor *et al* [10]). The sum of the components of the vector $|\Psi^{(2n)}\rangle$ is given by

$$\sum_{A \in W^{(2n)}} \Psi_A^{(2n)} = 3^{n/2} A_n.$$

Note that Hamiltonian (3) has a modified shift invariance. Indeed, it commutes with the operator

$$T' = T \exp \left[\frac{i\phi}{2} \left(\sigma_N^z - \frac{1}{N} \sum_{i=1}^N \sigma_i^z \right) \right]$$

where T is the operator of the right shift by a site. Our choice of the operator of modified shift invariance is dictated by the requirement $T'^N = 1$. Note that the operator T' commutes with the operator R' . It follows from these facts and from requirement (4) that in the case under consideration either $T'|\Psi^{(N)}\rangle = |\Psi^{(N)}\rangle$ or $T'|\Psi^{(N)}\rangle = -|\Psi^{(N)}\rangle$. It appears that for even $N \leq 12$ one has

$$T'|\Psi^{(N)}\rangle = |\Psi^{(N)}\rangle. \quad (13)$$

It is natural to suppose that this is so for any even N . It can be deduced from (13) that for any $k = 0, 1, \dots$

$$\sum_{A \in W^{(N)}} (\Psi_A^{(N)})^{3(2k+1)} = 0.$$

Let us proceed to the consideration of correlation functions. For any operator O we denote

$$\langle O \rangle_N = \frac{\langle \Psi^{(N)} | O | \Psi^{(N)} \rangle}{\langle \Psi^{(N)} | \Psi^{(N)} \rangle}.$$

It is evident that $\langle \sigma_{i_1}^z \dots \sigma_{i_k}^z \rangle_{2n}$ does not depend on the order of the operators σ_i^z . From (4) we obtain

$$\langle \sigma_{i_1}^z \dots \sigma_{i_{2k+1}}^z \rangle_{2n} = 0$$

for any $k = 0, 1, \dots$, and the equality (13) implies that

$$\langle \sigma_{i_1}^z \dots \sigma_{i_k}^z \rangle_{2n} = \langle \sigma_{i_{1+1}}^z \dots \sigma_{i_{k+1}}^z \rangle_{2n}.$$

To formulate our conjectures on correlation functions we introduce the operators

$$\alpha_i = (1 + \sigma_i^z)/2.$$

The analogue of conjecture 5 of [3] is

Conjecture 5.

$$\langle \alpha_i \alpha_{i+2} \rangle_{2n} = \frac{71n^4 - 19n^2 + 20}{16(4n^2 - 1)^2}.$$

Unlike the periodic case, this conjecture is a simple consequence of:

Conjecture 6. There is a simple formula for the correlation functions called in the book [13] the probabilities of formation of ferromagnetic string:

$$\frac{\langle \alpha_1 \alpha_2 \dots \alpha_{k-1} \rangle_{2n}}{\langle \alpha_1 \alpha_2 \dots \alpha_k \rangle_{2n}} = \frac{(2k-2)!(2k-1)!(2n+k-1)!(n-k)!}{(k-1)!(3k-2)!(2n-k)!(n+k-1)!}.$$

Note that the conjectured formulae for correlation functions have the same thermodynamic limit for both the twisted and periodic boundary conditions [3].

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