Spin chains and combinatorics

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Abstract

In this letter we continue the investigation of finite XXZ spin chains with periodic boundary conditions and odd number of sites, initiated in paper [1]. As it turned out, for a special value of the asymmetry parameter $\Delta = -1/2$ the Hamiltonian of the system has an eigenvalue, which is exactly proportional to the number of sites $E = -3N/2$. Using MATHEMATICA we have found explicitly the corresponding eigenvectors for $N \leq 17$. The obtained results support the conjecture of paper [1] that this special eigenvalue corresponds to the ground state vector. We make a lot of conjectures concerning the correlations of the model. Many remarkable relations between the wave function components are noticed. It is turned out, for example, that the ratio of the largest component to the least one is equal to the number of the alternating sing matrices.

The Hobbits of the Shire and of Bree had at this time, for probably a thousand years, adopted the Common Speech. They used it in their own manner freely and carelessly; though the more learned among them had still at their command a more formal language when occasion required.

(J. R. R. Tolkien)

The XXZ quantum spin chain model with periodic boundary conditions is one of the most popular integrable models which has been investigating by the Bethe Ansatz method during the last 35 years [3]. It is described by the Hamiltonian

$$H_{XXZ} = -\sum_{j=1}^{N} \left\{ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^z \sigma_{j+1}^z \right\}, \qquad \vec{\sigma}_{N+1} = \vec{\sigma}_1. \tag{1}$$

The advantages and shortcomings of the Bethe method are well known and we do not discuss them here. We do not discuss alternative methods elaborated by many people as well. We want only to draw attention of experts to some unique possibility to surpass these methods in one very special case.

As the starting point of our consideration we take the fact that for $\Delta = -1/2$ and odd number of sites $N = 2n + 1$, Hamiltonian (1) has an eigenvalue $E = -3N/2$. This fact was proved in paper [1]. The existence of such eigenvalue was earlier discovered numerically by Alcaraz, Barber and Batchelor [2]. Below we study the properties of the eigenvectors, corresponding to this special eigenvalue. We use the natural basis where all operators σ_j^z, $j = 1, \ldots, N$, are diagonal.

For the case $N = 3$ we have $2^N = 8$ states and it is not difficult to find all eigenvalues and eigenvectors. The results of calculations are described by Table 1, where $\omega = \exp(2\pi \mathrm{i}/3)$. Already this simplest case demonstrates some characteristic properties

Table 1: All eigenvectors for the case $N = 3$

$\lvert\Psi\rangle$	S_z	E
$\lvert\downarrow\downarrow\downarrow\rangle$	$-3/2$	$3/2$
$\lvert\uparrow\downarrow\downarrow\rangle + \lvert\downarrow\uparrow\downarrow\rangle + \lvert\downarrow\downarrow\uparrow\rangle$	$-1/2$	$-9/2$
$\lvert\uparrow\downarrow\downarrow\rangle + \omega\,\lvert\downarrow\uparrow\downarrow\rangle + \omega^2\,\lvert\downarrow\downarrow\uparrow\rangle$	$-1/2$	$3/2$
$\lvert\uparrow\downarrow\downarrow\rangle + \omega^2\,\lvert\downarrow\uparrow\downarrow\rangle + \omega\,\lvert\downarrow\downarrow\uparrow\rangle$	$-1/2$	$3/2$
$\lvert\downarrow\uparrow\uparrow\rangle + \lvert\uparrow\downarrow\uparrow\rangle + \lvert\uparrow\uparrow\downarrow\rangle$	$1/2$	$-9/2$
$\lvert\downarrow\uparrow\uparrow\rangle + \omega\,\lvert\uparrow\downarrow\uparrow\rangle + \omega^2\,\lvert\uparrow\uparrow\downarrow\rangle$	$1/2$	$3/2$
$\lvert\downarrow\uparrow\uparrow\rangle + \omega^2\,\lvert\uparrow\downarrow\uparrow\rangle + \omega\,\lvert\uparrow\uparrow\downarrow\rangle$	$1/2$	$3/2$
$\lvert\uparrow\uparrow\uparrow\rangle$	$3/2$	$3/2$

of the spectrum of Hamiltonian (1) and of its eigenvectors. First note that the operator

$$R = \prod_{j=1}^{N} \sigma_j^x,$$

reversing the z-axis projections of all spins, commutes with Hamiltonian (1), hence, every eigenvector has a partner with the same energy and the opposite value of S_z. In particular, the ground state is two-fold degenerate.

We see that our special eigenvalue corresponds to the ground state of the system. Then it is not surprising that it is unique for a fixed value of S_z and shift invariant. It is natural to start to suspect that this fact in not accidental and that our special eigenvalue corresponds to the ground state for an arbitrary odd N. Another indication supporting this hypothesis is that as was shown in paper [1], the eigenvalue $-3N/2$ occurs in the sectors with $S_z = \pm 1/2$ that resembles the value $S_z = 0$ occurring for the ground state in the case of an even N [4].

Let us proceed to larger values of N. Due to the symmetry described above it suffices to consider only positive or only negative values of S_z. For definiteness let us restrict ourselves to the case $S_z < 0$. Moreover, having in mind our hypothesis, we will consider only the shift invariant states.

The shift invariant eigenvectors for $N = 5$ and $S_z < 0$ are given in Table 2. A line above a vector means that we use the corresponding shift invariant combinations, for example,

$$\overline{\lvert\downarrow\downarrow\uparrow\downarrow\uparrow\rangle} = \lvert\downarrow\downarrow\uparrow\downarrow\uparrow\rangle + \lvert\downarrow\uparrow\downarrow\uparrow\downarrow\rangle + \lvert\uparrow\downarrow\uparrow\downarrow\downarrow\rangle + \lvert\downarrow\uparrow\downarrow\downarrow\uparrow\rangle + \lvert\uparrow\downarrow\downarrow\uparrow\downarrow\rangle.$$

The coincidence of the energy of the state with $S_z = -5/2$ and the energy of some state with $S_z = -1/2$ can be explained by the loop symmetry discovered by Korepanov [5] and recently elaborated by Deguchi, Fabricius and McCoy [6].

Table 2: All shift invariant eigenvectors for the case $N = 5$ and $S_z < 0$

$\lvert\Psi\rangle$	S_z	E
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\downarrow\rangle}$	$-5/2$	$5/2$
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\uparrow\rangle}$	$-3/2$	$-3/2$
$2\,\overline{\lvert\downarrow\downarrow\downarrow\uparrow\uparrow\rangle} - \overline{\lvert\downarrow\downarrow\uparrow\downarrow\uparrow\rangle}$	$-1/2$	$5/2$
$\overline{\lvert\downarrow\downarrow\downarrow\uparrow\uparrow\rangle} + 2\,\overline{\lvert\downarrow\downarrow\uparrow\downarrow\uparrow\rangle}$	$-1/2$	$-15/2$

Table 3 describes some shift invariant eigenvectors for the case $N = 7$. Actually we

Table 3: Some shift invariant eigenvectors for the case $N = 7$ and $S_z < 0$

$\lvert\Psi\rangle$	S_z	E
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle}$	$-7/2$	$7/2$
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\rangle}$	$-5/2$	$-5/2$
$2\,\overline{\lvert\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle} - \overline{\lvert\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle} + \overline{\lvert\downarrow\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle} - \overline{\lvert\downarrow\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\rangle}$	$-1/2$	$7/2$
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle} - 2\overline{\lvert\downarrow\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle} + \overline{\lvert\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle}$	$-1/2$	$3/2$
$\overline{\lvert\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle} - \overline{\lvert\downarrow\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\rangle}$	$-1/2$	$3/2$
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle} + \overline{\lvert\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle} + \overline{\lvert\downarrow\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\rangle} - \overline{\lvert\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle}$	$-1/2$	$-5/2$
$\overline{\lvert\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle} + 3\overline{\lvert\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\rangle} + 4\overline{\lvert\downarrow\downarrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle} + 3\overline{\lvert\downarrow\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\rangle} + 7\overline{\lvert\downarrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle}$	$-1/2$	$-21/2$

did not include there only the eigenvectors belonging to the sector with $S_z = -3/2$. The energy values in this sector are determined by the third order equation

$$8E^3 + 28E^2 - 298E - 411 = 0$$

which has no rational roots. The approximate values of the roots are $E \approx -7.5$, $E \approx -1.3$ and $E \approx 5.3$.

It is curious that the five states belonging to the sector $S_z = -1/2$ which for an arbitrary asymmetry parameter Δ lead to an equation of the fifth degree, have halfinteger energies for $\Delta = -1/2$. It is a manifestation of the general rule that in the case of $\Delta = -1/2$ the three spin wave energies for the states with zero momentum belong to the field $\mathbb{Q}$ of rationals extended with the root of unity $\exp(2\pi\mathrm{i}/(N-1))$. It will be, probably, published elsewhere but now we are interested in the ground state only.

We see that for $N = 5$ and $N = 7$ the special energy eigenvalue again corresponds to the ground state. So we confirm the following conjecture, formulated in paper [1] and supported by numerical calculations by Alcaraz, Barber and Batchelor [2]:

Conjecture 1 *The ground states of Hamiltonian* (1) *for an arbitrary odd N have the energy $E = -3N/2$ and $S_z = \pm 1/2$.*

If the above conjecture is true, then we have a real possibility to study the correlations for the finite periodic XXZ chains with $\Delta = -1/2$ and odd number of cites. Below we report a few conjectures related to the average over the states corresponding to the eigenvalue $-3N/2$.

Let us summarize the information related to the ground state for $N = 3, 5, 7$. We mark the components by the eigenvalues of the operators

$$a_j = (1 + \sigma_j^z)/2.$$

The nonzero wave function components are

$$\begin{array}{ll} N=3: & \psi_{001} = 1; \\ N=5: & \psi_{00011} = 1, \quad \psi_{00101} = 2; \\ N=7: & \psi_{0000111} = 1, \quad \psi_{0001101} = \psi_{0001011} = 3, \quad \psi_{0010011} = 4 \quad \psi_{0010101} = 7. \end{array}$$

All components not included in the list can be obtained by shifting. Notice that the components of the ground state are positive in accordance with the Perron–Frobenius theorem.

Let us continue the list. For $N = 9$ the components of the eigenvector with the energy $-27/2$ and $S_z = -1/2$ are

$$\begin{array}{llll} \psi_{000001111} = 1, & \psi_{000010111} = 4, & \psi_{000011011} = 6, & \psi_{000100111} = 7, \\ \psi_{000101011} = 17, & \psi_{000101101} = 14, & \psi_{000110011} = 12, & \psi_{001001011} = 21, \\ & \psi_{001010011} = 25, & \psi_{001010101} = 42. & \end{array}$$

We omit nonzero components which can be obtained by the reflection of the order of sites since this transformation is a symmetry of our state, as it is for the ground state. For example, we have

$$\psi_{000011101} = \psi_{000010111} = 4.$$

It is incredible at the turn of the millennium but up to this place the Computer was switched off! But the linear system for $N = 11$ contains 42 equation, so we invited the MATHEMATICA and obtained:

$$\begin{array}{llll} \psi_{00000011111} = 1, & \psi_{00000101111} = 5, & \psi_{00000110111} = 10, & \psi_{00001001111} = 11, \\ \psi_{00001010111} = 34, & \psi_{00001011011} = 41, & \psi_{00001011101} = 23, & \psi_{00001100111} = 30, \\ \psi_{00001101011} = 60, & \psi_{00010001111} = 14, & \psi_{00010010111} = 52, & \psi_{00010011011} = 73, \\ \psi_{00010011101} = 46, & \psi_{00010100111} = 75, & \psi_{00010101011} = 169, & \psi_{00010101101} = 128, \\ \psi_{00010110011} = 101, & \psi_{00011000111} = 42, & \psi_{00011001011} = 114, & \psi_{00100100111} = 81, \\ \psi_{00100101011} = 203, & \psi_{00100101101} = 174, & \psi_{00100110011} = 141, & \psi_{00101001011} = 226, \\ & \psi_{00101010011} = 260, & \psi_{00101010101} = 429. & \end{array}$$

It was a turning point of our work. The problem assumed a combinatorial character. The number 429 reminded us about the history of ASM conjecture [7]. The number of alternating sign $n \times n$ matrices is given by formula

$$A_n = \prod_{j=0}^{n-1} \frac{(3j+1)!}{(n+j)!}. \tag{2}$$

The sequence A_n goes as

$$1,\ 2,\ 7,\ 42,\ 429,\ 7436,\ 218348,\ 10850216, \ldots$$

The largest component of the wave functions for $N = 3, 5, 7, 9, 11$ goes in the same way! MATHEMATICA helped us to find components for $N = 13$, 15 and 17. For $N = 19$ the Computer was immersed in its calculations for too long, and we have lost patience. All the obtained results confirm

Conjecture 2 *If we chose the normalization of the state vector under consideration so that* $\psi_{0\ldots01\ldots1} = 1$ *then all other components are integer and the largest component is given by* $\psi_{0010101\ldots01} = A_n$.

Moreover we obtained that the components of the state vector are positive. Therefore, in accordance with the Perron–Frobenius theorem the special energy eigenvalue corresponds to the ground state at least in the sectors with $S_z = \pm 1/2$.

Now we are analyzing the obtained information and can already formulate some conjectures which are verified for odd $N \leq 17$.

For calculations of correlations one needs to know the norm of the ground state. For $N = 2n + 1$ we denote it by $\mathcal{N}_n$. The results of calculations looks as

$$\mathcal{N}_1 = \sqrt{3}, \quad \mathcal{N}_2 = 5, \quad \mathcal{N}_3 = 14\sqrt{3}, \quad \mathcal{N}_4 = 198, \quad \ldots$$

They are in agreement with

Conjecture 3 *If we chose the normalization so that* $\psi_{0\ldots01\ldots1} = 1$ *the norm of our state is*

$$\mathcal{N}_n = \frac{\sqrt{3^n}}{2^n} \frac{2 \cdot 5 \ldots (3n-1)}{1 \cdot 3 \ldots (2n-1)} A_n.$$

It is curious that the sequence of the linear sums of the components also display the simple parametrization.

Conjecture 4 *The sum of all components of the state vector under consideration is equal to* $(\sqrt{3})^n \mathcal{N}_n$.

As was shown in paper [1], the simplest nontrivial correlations are described by the formula

$$\langle \sigma_j^z \sigma_{j+1}^z \rangle = -\frac{1}{2} + \frac{3}{2(2n+1)^2}.$$

This implies that

$$\langle a_j \, a_{j+1} \rangle = \frac{(n-1)n}{2(2n+1)^2}.$$

Our results are in agreement with this formula.

We have also a fit for the next 2-spin correlations:

Conjecture 5

$$\langle a_j \, a_{j+2} \rangle = \frac{(n-1)}{4(2n-1)(2n+1)^2(2n+3)} \left[\frac{71}{4} n^3 + \frac{149}{4} n^2 + 18n + 9 \right].$$

In spite of its ugly look the above formula possesses some hidden symmetry, as well as the next one.

Conjecture 6 *There is a simple formula for the correlations called the Probabilities of Formation of Ferromagnetic String* [8]*:*

$$\frac{\langle a_1\, a_2\, \dots\, a_{k-1}\rangle}{\langle a_1\, a_2\, \dots\, a_k\rangle} = \frac{(2k-2)!\,(2k-1)!\,(2n+k)!\,(n-k)!}{(k-1)!\,(3k-2)!\,(2n-k+1)!\,(n+k-1)!}.$$

If this conjecture is correct then we obtain in the thermodynamic limit

$$\langle a_1\, a_2\, \dots\, a_k\rangle = \left(\frac{\sqrt{3}}{2}\right)^{3k^2} \prod_{m=1}^{k} \frac{\Gamma(m-1/3)\Gamma(m+1/3)}{\Gamma(m-1/2)\Gamma(m+1/2)}.$$

Using the standard properties of $\Gamma(x)$ we find an asymptotic of this correlator for large values of k

$$\langle a_1\, a_2\, \dots\, a_k\rangle \approx c \left(\frac{\sqrt{3}}{2}\right)^{3k^2} k^{-\frac{5}{36}},$$

where

$$c = \exp\left[\int_0^\infty \left(\frac{5}{36}\exp(-t) - \frac{\sinh(5t/12)\sinh(t/12)}{\sinh^2(t/2)}\right)\frac{dt}{t}\right] \approx 0.77466966.$$

The last conjecture touches the both ground states. The additional transverse magnetic field which is described by

$$\Delta H = h \sum_{j=1}^{N} \sigma_j^x,$$

splits the energies of the two ground states. In the first order the splitting is determined by the matrix element

$$M = \langle S_z = 1/2 | \sigma_j^x | S_z = -1/2\rangle.$$

Our data are in agreement with

Conjecture 7

$$(2n+1)\; M = \frac{4\cdot 7\cdot \dots\, (3n+1)}{2\cdot 5\cdot \dots\, (3n-1)}.$$

In conclusion we would like to concentrate the reader's attention on the appearance in our investigation of many combinatorial relations and remarkable combinatorial numbers. We consider it as an indication on the existence of rather simple expressions for the components of the ground state eigenvector of the model.

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