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Large- N behaviour of string solutions in the Heisenberg model

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Abstract

We investigate the large- N behaviour of the complex solutions for the two-magnon system in the $S = 1/2$ Heisenberg XXZ model. The Bethe ansatz equations are numerically solved for the string solutions with a new iteration method. Clear evidence of the violation of the string configurations is found at $N = 22, 62, 121, 200, 299, 417$, but the broken states are still Bethe states. The number of Bethe states is consistent with the exact diagonalization, except for one singular state.

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1. Introduction

In 1931, Bethe presented a unique and ingenious way of solving one-dimensional Heisenberg model with spin $S = 1/2$ systems [1, 2]. The structure of the Bethe ansatz solutions has been studied quite extensively. Since the Bethe ansatz method has a history of many years, the fundamental properties of the Bethe ansatz solution for the Heisenberg XXZ model are well understood by now [3–7]. However, the completeness of the Bethe ansatz solutions is still discussed actively [8–10]. Bethe ansatz solutions contain complex solutions whose rapidities are complex values. For these solutions, Bethe proposed the *string hypothesis*. He assumed the shape of the complex solutions which are called ‘string solutions’, and showed that the real solutions together with such complex solutions give the correct number of states [1]. Therefore, it is widely believed that the completeness of Bethe’s state holds true.

In the two-magnon system, the solutions are parametrized by two integer numbers m_1 and m_2 . The string solutions can be classified into two different types, depending on the parity of $m_1 + m_2$ in the two-magnon state. In fact, the behaviour of the wavefunction for the two string solutions is quite different. The string solutions with odd parity of $m_1 + m_2$ were first discussed by Bethe, and since then they have been discussed quite extensively. In particular, Essler,

Korepin and Schoutens (EKS) carried out a careful study of the string solutions. Here, we call this type of string the ‘EKS-string’ as we define later in detail. Recently, it has been found that these EKS-string solutions break down to two real solutions at $N = 22, 62, 121, \dots$ [12–14], which are partly predicted by Essler, Korepin and Schoutens. On the other hand, there are other types of complex solutions which are treated by Vladimirov [11]. These string solutions have even parity of $m_1 + m_2$, but their behaviour is quite different from the EKS-strings. Here, we call them ‘V-string’. According to the string hypothesis, the imaginary part of the string is $1/2$. However, Vladimirov shows that the imaginary part of the V-strings behaves as \sqrt{N} .

In this paper, we present the large- N behaviour of the string solutions of the Bethe ansatz equations for the two-magnon system. Here, we have solved the Bethe ansatz equations numerically up to quite a large number of sites N . The numerical evaluation has some difficulties for the complex solutions in the Bethe ansatz equations. A simple iteration method cannot give any convergent results, and thus we have to develop a new way to solve them. This is what we have achieved here as we discuss later in detail. The solutions are compared with those of the exact diagonalization method up to $N = 180$. Here, we indeed confirm the violation of the EKS-strings up to $N = 417$. Further, they are *not* out of the Bethe ansatz solutions, and therefore, the number of states is unchanged. In addition, we confirm that the behaviour of the V-string rapidity, predicted by the $1/N$ expansion method [11], is indeed consistent with our numerical solutions.

The paper is organized as follows. In the following section, we briefly explain the solutions of the Bethe ansatz equations. In section 3, we present a new iteration method for solving the Bethe equations numerically. In section 4, the string solutions for large- N cases are discussed and compared with the predictions of the $1/N$ expansion method. Section 5 summarizes what we have clarified.

2. The solutions of the Bethe ansatz equations

The Heisenberg XXZ model with spin $1/2$ is a model which is the most frequently studied of all the models of the spin systems. It is solved by the Bethe ansatz technique. Here, we briefly describe the Heisenberg model and the Bethe ansatz solutions. The XXZ model is described by the following Hamiltonian,

$$H = J \sum_{i=1}^N (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) = \frac{J}{2} \sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + 2\Delta S_i^z S_{i+1}^z) \quad (1)$$

where S_i^a is a spin operator at the site i and S_i^- (S_i^+) flips down (up) the spin, and Δ is the anisotropic parameter. The periodicity $S_{N+i} = S_i$ is assumed. For the XXX model, we take $\Delta = 1$. This Hamiltonian can be diagonalized by the following Bethe state [1, 2] for the two-magnon system,

$$|\Psi_2\rangle = \sum_{x_1 < x_2} A(x_1, x_2) S_{x_1}^- S_{x_2}^- |0\rangle \quad (2)$$

where $|0\rangle$ is the ferromagnetic state with all spins up. The coefficient $A(x_1, x_2)$ is assumed to be of the following shape,

$$A(x_1, x_2) = e^{ik_1 x_1 + ik_2 x_2} + e^{ik_2 x_1 + ik_1 x_2} e^{-i\varphi} \quad (3)$$

and must satisfy

$$A(x_j, x_j) + A(x_j + 1, x_j + 1) - 2A(x_j, x_j + 1) = 0. \quad (4)$$

Therefore, the phase shift φ should satisfy the following equation:

$$\cot \frac{\varphi}{2} = \frac{\Delta \sin \frac{k_1 - k_2}{2}}{\cos \frac{k_1 + k_2}{2} - \Delta \cos \frac{k_1 - k_2}{2}} \tag{5}$$

where φ is taken to be $-\pi \leq \varphi \leq \pi$. Further, imposing the periodic boundary conditions, we have

$$k_1 N + \varphi = 2\pi m_1 \tag{6}$$

$$k_2 N - \varphi = 2\pi m_2 \tag{7}$$

where m_1 and m_2 are integers running between 0 and $N - 1$. Without loss of generality, we can take $m_1 \leq m_2$. In this case, the energy eigenvalue of the Hamiltonian can be written as

$$E/J = \sum_{j=1}^2 \cos k_j + \Delta \left(\frac{N}{4} - 2 \right). \tag{8}$$

We can define the rapidity as

$$\lambda_j = -\frac{1}{2} \cot \frac{k_j}{2}. \tag{9}$$

In this case, the energy is given by

$$E/J = -\frac{1}{2} \sum_{j=1}^2 \frac{1}{\lambda_j^2 + 1/4} + \Delta \left(\frac{N}{4} - 2 \right) + 2. \tag{10}$$

In order to obtain the energy eigenvalues of the Hamiltonian, one has to solve equations (5), (6) and (7). Here, we show the rapidity and the energy in the case of $N = 8$ and $\Delta = 1$ for simplicity. We must solve the equation

$$\cos \frac{\pi}{N} (m_1 + m_2) \cos \left(\frac{NK}{2} - \frac{\pi}{2} (m_1 - m_2) \right) = \cos \left(\frac{N-2}{4} K - \frac{\pi}{2} (m_1 - m_2) \right) \tag{11}$$

where $K = (k_1 - k_2)/2$. This equation can be solved analytically once we specify the values of m_1 and m_2 . It is difficult to prove the completeness of the Bethe ansatz solutions. Therefore, we must carefully treat the Bethe ansatz equation whose solutions are indeed the answer to the model.

In table 1, we show the calculated results of the energies for $N = 8$ with the two down spins together with the energies by the exact diagonalization for $\Delta = 1$. The detailed method of solving the Bethe equations numerically will be given in section 3.

As can be seen from table 1, there is one state, denoted by *, which cannot be reproduced by the Bethe ansatz. The configurations of these states are different for different values of Δ . Here, we only show the results for the $\Delta = 1$ case. For other values of Δ , we only make a comment here. We have the real solution for $\Delta = 1$ in category I, which is defined in [3]. The string solutions appear for categories II and III. For $\Delta = 2$, there is an irregular solution at $(m_1, m_2) = (0, 7)$. Even though the element belongs to category I, the solution is a string. We have a similar configuration for the case $\Delta > 1$. On the other hand, there is no complex solution for $\Delta = 1/2$ at $N = 8$. In what follows, we will only discuss the $\Delta = 1$ case. The general Δ cases will be treated elsewhere.

Now, there is a state which cannot be reproduced by the Bethe ansatz solution for $\Delta = 1$. We can easily verify that the energy of this state is given by

$$E/J = \Delta \left(\frac{N}{4} - 1 \right). \tag{12}$$

Table 1. The energies E_{exact} and E_{Bethe} , which are solved by the exact diagonalization and by the Bethe ansatz method, are presented for the $N = 8$ and $\Delta = 1$ case. The symbol * means that there is no corresponding state in the Bethe ansatz method.

| E_{exact}/J | E_{Bethe}/J | (m_1, m_2) | k_1 | k_2 | φ |
|----------------------|---------------------------------|--------------|---------------------|---------------------|-----------------|
| -1.801 938 | $-2 \cos \frac{\pi}{7}$ | (3, 5) | $6\pi/7$ | $8\pi/7$ | $6\pi/7$ |
| -1.267 035 | -1.267 035 | (2, 4) | 0.6035π | 0.8965π | 0.8279π |
| | | (4, 6) | 1.1035π | 1.3965π | 0.8279π |
| -1.144 123 | $-\frac{\sqrt{10}+\sqrt{2}}{4}$ | (2, 5) | 0.5875π | 1.1625π | 0.7003π |
| | | (3, 6) | 0.8375π | 1.4125π | 0.7003π |
| -0.445 0419 | $-2 \cos \frac{3}{7}\pi$ | (2, 6) | $4\pi/7$ | $10\pi/7$ | $4\pi/7$ |
| -0.437 0160 | $-\frac{\sqrt{10}-\sqrt{2}}{4}$ | (1, 4) | 0.3184π | 0.9316π | 0.5475π |
| | | (4, 7) | 1.0684π | 1.6816π | 0.5475π |
| -0.258 6520 | -0.258 6520 | (1, 5) | 0.3085π | 1.1915π | 0.4684π |
| | | (3, 7) | 0.8085π | 1.6915π | 0.4684π |
| 0 | 0 | (0, 4) | 0 | π | 0 |
| | | (1, 3) | $\pi/3$ | $2\pi/3$ | $2\pi/3$ |
| | | (5, 7) | $4\pi/3$ | $5\pi/3$ | $2\pi/3$ |
| 0.292 8932 | $\frac{2-\sqrt{2}}{2}$ | (0, 3) | 0 | $3\pi/4$ | 0 |
| | | (0, 5) | 0 | $5\pi/4$ | 0 |
| 0.437 0160 | $\frac{\sqrt{10}-\sqrt{2}}{4}$ | (1, 6) | 0.2990π | 1.4510π | 0.3920π |
| | | (2, 7) | 0.5490π | 1.7010π | 0.3920π |
| 1.0 | 1 | (0, 2) | 0 | $\pi/2$ | 0 |
| | | (0, 6) | 0 | $3\pi/2$ | 0 |
| 1.0 | * | * | | | |
| 1.144 123 | $\frac{\sqrt{10}+\sqrt{2}}{4}$ | (1, 2) | $3\pi/8 + 0.9578i$ | $3\pi/8 - 0.9578i$ | $\pi + 7.6626i$ |
| | | (6, 7) | $13\pi/8 + 0.9578i$ | $13\pi/8 - 0.9578i$ | $\pi + 7.6626i$ |
| 1.246 980 | $-2 \cos \frac{5}{7}\pi$ | (1, 7) | $2\pi/7$ | $12\pi/7$ | $2\pi/7$ |
| 1.525 687 | 1.525 687 | (1, 1) | $\pi/4 + 0.3945i$ | $\pi/4 - 0.3945i$ | $3.1559i$ |
| | | (7, 7) | $7\pi/4 + 0.3945i$ | $7\pi/4 - 0.3945i$ | $3.1559i$ |
| 1.707 107 | $\frac{2+\sqrt{2}}{2}$ | (0, 1) | 0 | $\pi/4$ | 0 |
| | | (0, 7) | 0 | $7\pi/4$ | 0 |
| 2.0 | 2 | (0, 0) | 0 | 0 | 0 |

The corresponding state is

$$|\text{non-Bethe}\rangle = \sum_{i=1}^N (-)^i S_i^- S_{i+1}^- |0\rangle. \quad (13)$$

Note that the *kinetic term* of this state is null,

$$\sum_i (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) |\text{non-Bethe}\rangle = 0. \quad (14)$$

Thus, we cannot describe this state in the Bethe ansatz equation because equation (5) is not valid for this case any more. We note here that this state is not reproduced by the algebraic Bethe ansatz at the isotropic point either [15].

Bethe suggested that there is a string solution whose imaginary part is infinity [1]. However, the wavefunction is divergent. For appropriate normalization, we get the wavefunction given as equation (13). Therefore, the wavefunction (13) corresponds to the singular Bethe state.

We comment on the degeneracy of the energy states. Suppose that the k_1, k_2 are solutions for the configuration (m_1, m_2) ($1 \leq m_1 \leq m_2 \leq N - 1$) with the phase φ . The Bethe equations are

$$k_1 N + \varphi = 2\pi m_1 \quad k_2 N - \varphi = 2\pi m_2. \tag{15}$$

Now we consider the configuration $(N - m_2, N - m_1)$ with k'_1, k'_2, φ' . We can easily show that two states have the same energy if the following equations are satisfied:

$$k'_1 + k'_2 = 4\pi - (k_1 + k_2) \quad k'_1 - k'_2 = k_1 - k_2 \quad \varphi' = \varphi. \tag{16}$$

Note that

$$k'_i = k_i \quad (i = 1, 2) \quad \text{for } m_1 + m_2 = N. \tag{17}$$

In this case, there is no pair and the Bethe state is a single state. For the $(0, m_2)$ ($1 \leq m_2 \leq N - 1$) case, the configuration $(0, N - m_2)$ is a solution with the same energy as the configuration $(0, m_2)$ when

$$k'_1 + k'_2 = 2\pi - (k_1 + k_2) \quad k'_1 - k'_2 = -(k_1 - k_2) - 2\pi \quad \varphi' + \varphi = 0. \tag{18}$$

3. New iteration method

The Bethe ansatz equations (5), (6) and (7) can be solved by the iteration method even for the large- N cases. The convergence of the iteration method is good for the normal cases, but the complex solutions cannot be obtained easily by the simple-minded iteration method. Here, we present a somewhat different way of numerically solving the Bethe equations. But before going to the new method, we briefly explain the usual iteration method. The φ in equation (5) can be written as

$$\varphi = 2 \cot^{-1} \frac{\Delta \sin \frac{k_1 - k_2}{2}}{\cos \frac{k_1 + k_2}{2} - \Delta \cos \frac{k_1 - k_2}{2}} \equiv X(\varphi). \tag{19}$$

The usual iteration method is as follows,

$$\varphi^{(i)} = X(\varphi^{(i-1)}) \tag{20}$$

where we start from some initial value of $\varphi^{(0)}$. k_1 and k_2 are given in equations (6) and (7). As mentioned above, this procedure works well for the normal cases. But for the complex solutions, it does not work.

In this paper, we show a new way of solving the complex solutions. First, we define a new variable v by

$$\varphi = iv \quad \text{for } (m, m) \quad (\text{V-string}) \tag{21}$$

$$\varphi = \pi + iv \quad \text{for } (m, m + 1) \quad (\text{EKS-string}) \tag{22}$$

where v is taken to be real. For the V-string case (m, m) , we obtain

$$\coth \frac{v}{2} = \frac{-\Delta \sinh \frac{v}{N}}{\cos \frac{2m\pi}{N} - \Delta \cosh \frac{v}{N}} \quad \sinh \frac{v}{2} = \frac{\cos \frac{2m\pi}{N} - \Delta \cosh \frac{v}{N}}{-\Delta \sinh \frac{v}{N}} \cosh \frac{v}{2} \equiv X(v)$$

$$v = 2 \ln \left(X + \sqrt{X^2 + 1} \right).$$

Therefore, the iteration equation becomes

$$v^{(i)} = 2 \ln \left(X + \sqrt{X^2 + 1} \right) \Big|_{v=v^{(i-1)}}. \tag{23}$$

On the other hand, for the case of the EKS-string $(m, m + 1)$, we have

$$\begin{aligned} \tanh \frac{v}{2} &= \frac{-\Delta \sinh \frac{v}{N}}{\cos \frac{(2m+1)\pi}{N} - \Delta \cosh \frac{v}{N}} & \cosh \frac{v}{2} &= \frac{\cos \frac{(2m+1)\pi}{N} - \Delta \cosh \frac{v}{N}}{-\Delta \sinh \frac{v}{N}} \sinh \frac{v}{2} \equiv Y(v) \\ v &= 2 \ln \left(Y + \sqrt{Y^2 - 1} \right). \end{aligned}$$

Therefore, the iteration equation becomes

$$v^{(i)} = 2 \ln \left(Y + \sqrt{Y^2 - 1} \right) \Big|_{v=v^{(i-1)}}. \tag{24}$$

We can carry out the iteration procedure a million times, and obtain good convergent results. In this way, this iteration method gives complete solutions, and thus we can find all of the string solutions of the V-string as well as the EKS-string. With this method, we can find the string solutions up to $N \simeq 5000$.

4. String solutions for large N

Next, we discuss the properties of the string solutions. For the string hypothesis, the complex solutions are given for an M -magnon system by

$$\lambda_j = x + i \left(\frac{M+1}{2} - j \right) + O(e^{-\delta N}) \quad (j = 1, 2, \dots, M) \tag{25}$$

where x is the same real part of the complex roots λ_j , and δ is a positive parameter. According to the string hypothesis, the imaginary part y of the string at large N is given as

$$y \rightarrow \frac{1}{2} \tag{26}$$

for the two-magnon case ($M = 2$). On the other hand, Vladimirov predicts [11] the non-string-type complex solutions by making use of the $1/N$ expansion method. Defining the real and imaginary parts of the rapidity by $\lambda = x \pm iy$, they can be expressed as

$$x = \frac{N}{\pi \ell} \left(1 - \frac{1}{N} - \frac{\pi^2 \ell^2}{6N^2} + \dots \right) \quad y = \frac{\sqrt{N}}{\pi \ell} \left[1 + \frac{1}{N} \left(\frac{\pi^2 \ell^2}{24} - \frac{1}{2} \right) + \dots \right] \tag{27}$$

where $\ell = 2, 4, 6, \dots \leq \sqrt{N}$. For large N , they behave as

$$x \sim N \quad y \sim \sqrt{N}. \tag{28}$$

In table 2, we show the complex solutions of the XXX model for several cases of N . The Vladimirov solutions are given in the following configurations,

$$(m_1, m_2) = (r, r) \quad r = 1, 2, \dots, \left[\frac{\sqrt{N}}{2} \right] \tag{29}$$

where $[x]$ denotes the maximum integer n for $n \leq x$ (Gauss's symbol). In figures 1 and 2, we show the large- N behaviour of the imaginary part and the real part of the complex solutions, respectively. We can see that the large- N behaviour of the configuration for $(m_1, m_2) = (1, 1), (2, 2)$ is indeed consistent with equation (28).

On the other hand, the large- N behaviour of the configurations for the $m_2 = m_1 + 1$ case is different. We show the behaviour of the imaginary part and the real part of the complex solutions in figures 3 and 4. There are branch points where the string solutions break down.

Table 2. The energies E_{exact} and the string solutions and non-string-type solutions which are solved numerically for the XXX model ($\Delta = 1$). The variable λ_{Vlad} is the Vladimirov prediction.

| N | E_{exact}/J | (m_1, m_2) | λ | λ_{Vlad} |
|------------|----------------------|--------------------------------|--------------------------------|--|
| 12 | 2.762 259 03 | (1, 1) | $1.651\ 0879 \pm 0.619\ 417i$ | $1.653\ 8681 \pm 0.617\ 998i$ ($\ell = 2$) |
| | 2.250 545 60 | (2, 2) | $0.576\ 9306 \pm 0.500\ 242i$ | – |
| | ⋮ | ⋮ | ⋮ | – |
| | 2.490 9371 | (1, 2) | $1.018\ 4604 \pm 0.480\ 8314i$ | – |
| | 2.066 9861 | (2, 3) | $0.267\ 9495 \pm 0.499\ 9999i$ | – |
| 22 | ⋮ | ⋮ | ⋮ | – |
| | 5.423 3830 | (1, 1) | $3.291\ 3953 \pm 0.791\ 3153i$ | $3.291\ 8067 \pm 0.791\ 0191i$ ($\ell = 2$) |
| | 5.210 0924 | (2, 2) | $1.543\ 4373 \pm 0.519\ 0729i$ | $1.553\ 1493 \pm 0.515\ 5661i$ ($\ell = 4$) |
| | 4.928 9111 | (3, 3) | $0.866\ 4011 \pm 0.500\ 090i$ | – |
| | ⋮ | ⋮ | ⋮ | – |
| | 5.070 4584 | (2, 3) | $1.155\ 9456 \pm 0.497\ 8173i$ | – |
| | 4.792 2902 | (3, 4) | $0.642\ 6630 \pm 0.499\ 9987i$ | – |
| 4.579 3732 | (4, 5) | $0.293\ 6265 \pm 0.500\ 0000i$ | – | |
| 60 | ⋮ | ⋮ | ⋮ | – |
| | 14.989 239 | (1, 1) | $9.372\ 2865 \pm 1.257\ 6148i$ | $9.372\ 3056 \pm 1.257\ 5917i$ ($\ell = 2$) |
| | 14.957 218 | (2, 2) | $4.656\ 6352 \pm 0.688\ 1097i$ | $4.657\ 1019 \pm 0.687\ 560i$ ($\ell = 4$) |
| | 14.904 929 | (3, 3) | $3.064\ 1980 \pm 0.539\ 7430i$ | $3.067\ 3519 \pm 0.537\ 2569i$ ($\ell = 6$) |
| | 14.834 704 | (4, 4) | $2.244\ 1546 \pm 0.504\ 2061i$ | – |
| | ⋮ | ⋮ | ⋮ | – |
| | 14.931 927 | (2, 3) | $3.793\ 5172 \pm 0.129\ 7153i$ | – |
| | 14.871 226 | (3, 4) | $2.612\ 1248 \pm 0.481\ 2710i$ | – |
| 14.793 839 | (4, 5) | $1.963\ 1184 \pm 0.499\ 0019i$ | – | |
| 100 | ⋮ | ⋮ | ⋮ | – |
| | 24.996 095 | (1, 1) | $15.745\ 726 \pm 1.610\ 3627i$ | $15.745\ 730 \pm 1.610\ 3563i$ ($\ell = 2$) |
| | 24.984 411 | (2, 2) | $7.856\ 0250 \pm 0.848\ 3587i$ | $7.856\ 1233 \pm 0.848\ 1972i$ ($\ell = 4$) |
| | 24.965 063 | (3, 3) | $5.216\ 2758 \pm 0.620\ 5981i$ | $5.216\ 9764 \pm 0.619\ 5799i$ ($\ell = 6$) |
| | 24.938 297 | (4, 4) | $3.885\ 7124 \pm 0.533\ 9379i$ | $3.888\ 3774 \pm 0.531\ 4536i$ ($\ell = 8$) |
| | 24.904 572 | (5, 5) | $3.075\ 6442 \pm 0.506\ 2334i$ | $3.081\ 6823 \pm 0.507\ 4819i$ ($\ell = 10$) |
| | 24.864 499 | (6, 6) | $2.525\ 4416 \pm 0.500\ 6816i$ | – |
| | ⋮ | ⋮ | ⋮ | – |
| | 24.952 091 | (3, 4) | $4.504\ 2779 \pm 0.335\ 3532i$ | – |
| | 24.922 034 | (4, 5) | $3.447\ 7639 \pm 0.479\ 7970i$ | – |
| | 24.885 222 | (5, 6) | $2.778\ 4399 \pm 0.497\ 6799i$ | – |
| ⋮ | ⋮ | ⋮ | – | |

At the branch point, the imaginary part is close to zero, and the real part is divided into two parts. However, the broken string becomes two real solutions in the Bethe ansatz equation and thus these broken states are still degenerate, which is shown in table 3. In table 4, we list the configurations for the complex solutions.

In figure 5, the minimum number of m_1 and the number of sites N are given. The number of the string does not increase linearly for N . Note that, in both cases, there are string solutions whose imaginary part is $1/2$. However, the value of the imaginary part starts to deviate from $1/2$ when the value of the number of sites N increases, and finally becomes zero for sufficiently large values of N .

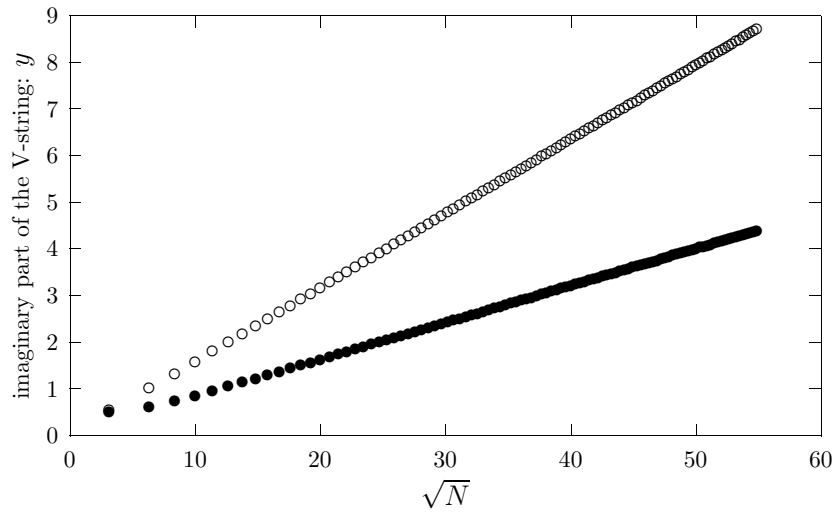


Figure 1. The large- N behaviour of the V-string solutions for the XXX model ($\Delta = 1$). Plot of the imaginary part of the string against \sqrt{N} for $(m_1, m_2) = (1, 1)$ (plotted with the symbol \circ) and $(m_1, m_2) = (2, 2)$ (plotted with the symbol \bullet).

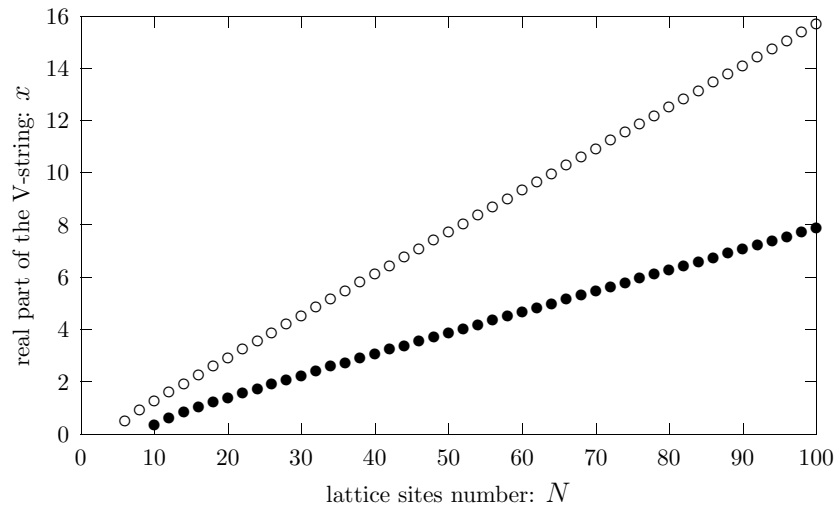


Figure 2. The large- N behaviour of the V-string solutions for the XXX model ($\Delta = 1$). Plot of the real part of the string against the number of sites N for $(m_1, m_2) = (1, 1)$ (plotted with the symbol \circ) and $(m_1, m_2) = (2, 2)$ (plotted with the symbol \bullet).

Finally, the string configurations for the XXX model ($\Delta = 1$) are classified by the large- N behaviour. In [14], Ilakovac *et al* distinguish the string solution in terms of the parity of $m_1 + m_2$. They call the string solutions *s*-string for the odd-parity case and *c*-string for the even-parity case. The string solutions are given by

$$\text{V-string (c-string): } (m_1, m_2) = (r, r), (N - r, N - r) \quad \left(0 < r < \frac{N}{4}\right) \quad (30)$$

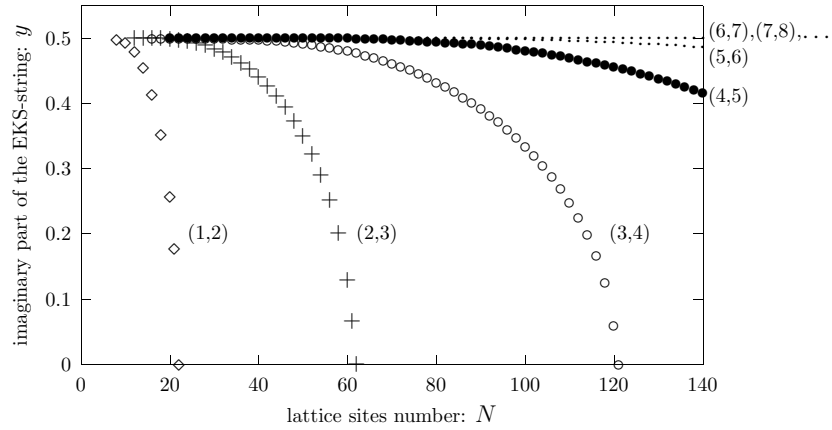


Figure 3. The large- N behaviour of the EKS-string solutions for the XXX model ($\Delta = 1$). Plot of the imaginary part of the string against the number of sites N for the $m_2 = m_1 + 1$ case.

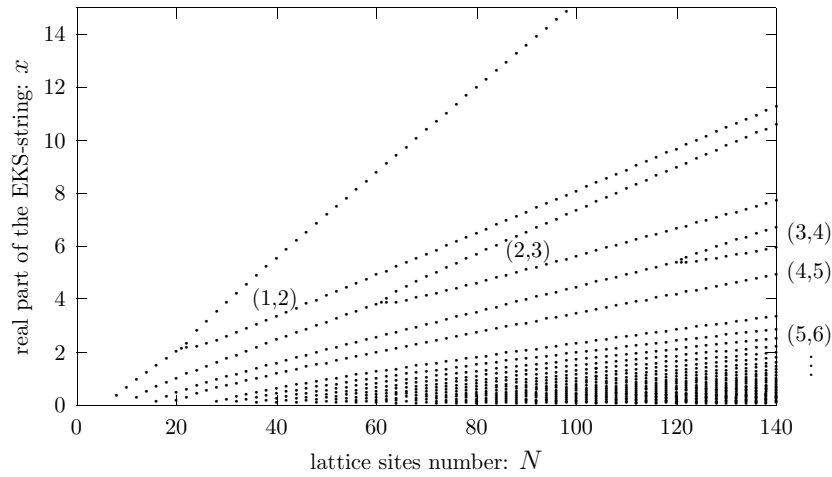


Figure 4. The large- N behaviour of the EKS-string solutions for the XXX model ($\Delta = 1$). Plot of the real part of the string against the number of sites N for the $m_2 = m_1 + 1$ case.

$$\text{EKS-string } (s\text{-string}): \quad (m_1, m_2) = (s, s + 1), (N - s - 1, N - s) \quad \left(s_0 < s < \frac{N}{4} \right) \tag{31}$$

where r, s are integers and s_0 is the minimum of m_1 . The distribution of s_0 is given by figure 5. For large N , we have

$$s_0 \sim 0.3347N^{0.4934} \sim \sqrt{N}. \tag{32}$$

Therefore, we can estimate the ratio of the number of the string N_{string} to the total states $N_{\text{total}} = N(N - 1)/2$ as

$$\frac{N_{\text{string}}}{N_{\text{total}}} \sim \frac{2}{N} - \frac{2}{N\sqrt{N}}. \tag{33}$$

Table 3. The energies and the string solutions near the breaking point for the XXX model. The symbol * means that the exact diagonalization is not possible.

| (m_1, m_2) | N | E_{exact}/J | E_{Bethe}/J | λ |
|--------------|-----|----------------------|----------------------|-----------------------------------|
| (1, 2) | 21 | 5.051 937 73 | 5.051 937 73 | $2.176\,6735 \pm 0.178\,889\,55i$ |
| | 22 | 5.319 109 54 | 5.319 109 54 | 2.372 7865 2.228 4619 |
| (2, 3) | 61 | 15.184 0740 | 15.184 0740 | $3.860\,7743 \pm 0.066\,412\,34i$ |
| | 62 | 15.436 1213 | 15.436 1213 | 4.019 3617 3.836 6348 |
| (3, 4) | 120 | 29.966 5138 | 29.966 5138 | $5.440\,8068 \pm 0.059\,899\,96i$ |
| | 121 | 30.217 0566 | 30.217 0566 | 5.539 9897 5.435 1240 |
| (4, 5) | 199 | * | 49.729 8474 | $7.026\,0588 \pm 0.044\,648\,58i$ |
| | 200 | * | 49.980 0466 | 7.104 5560 7.019 490 |

Table 4. The configurations and the number of the states N_{string} of the complex solutions for the XXX model ($\Delta = 1$). Here, we list for $m_1, m_2 < N/2$ cases. The other cases are given by taking $(N - m_2, N - m_1)$. The boldface shows the missing points of the string.

| N | (m_1, m_2) | $N_{\text{string}}/2$ |
|------------|-------------------|-----------------------|
| 8 | (1, 1) | (1, 2) 2 |
| 10 | (1, 1), (2, 2) | (1, 2) 3 |
| | | ⋮ |
| 20 | (1, 1)–(4, 4) | (1, 2)–(4, 5) 8 |
| 22 | (1, 1)–(5, 5) | (2, 3)–(4, 5) 8 |
| | | ⋮ |
| 60 | (1, 1)–(14, 14) | (2, 3)–(14, 15) 27 |
| 62 | (1, 1)–(15, 15) | (3, 4)–(14, 15) 27 |
| | | ⋮ |
| 120 | (1, 1)–(29, 29) | (3, 4)–(29, 30) 56 |
| 121 | (1, 1)–(29, 29) | (4, 5)–(29, 30) 55 |
| | | ⋮ |
| 199 | (1, 1)–(49, 49) | (4, 5)–(48, 49) 94 |
| 200 | (1, 1)–(49, 49) | (5, 6)–(48, 49) 94 |
| | | ⋮ |
| 298 | (1, 1)–(74, 74) | (5, 6)–(73, 74) 143 |
| 299 | (1, 1)–(73, 73) | (6, 7)–(73, 74) 142 |
| | | ⋮ |
| 416 | (1, 1)–(103, 103) | (6, 7)–(103, 104) 201 |
| 417 | (1, 1)–(103, 103) | (7, 8)–(103, 104) 200 |
| | | ⋮ |

If the string violation does not occur, the ratio is

$$\frac{N_{\text{string}}}{N_{\text{total}}} \sim \frac{2}{N} - \frac{6}{N^2}. \quad (34)$$

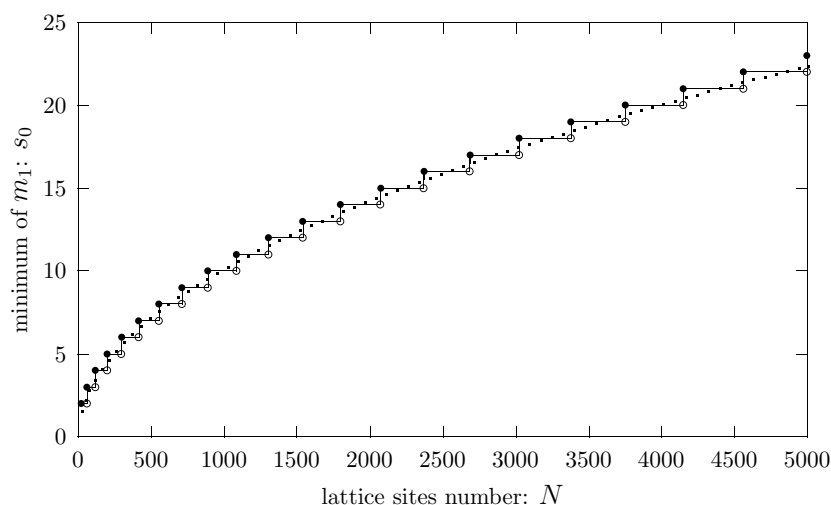


Figure 5. Plot of the minimum(s_0) of m_1 against the number of sites N for the $m_2 = m_1 + 1$ case in the XXX model. The symbol \circ means that the point is excluded. The fitting function which is denoted by the dotted line is given by $s_0 \sim N^{0.4934}$.

5. Conclusion

We have presented systematic calculations of the large- N behaviour in the spin-1/2 Heisenberg XXX model. Here, we have developed a new iteration method which enables us to evaluate all of the complex solutions. Though we have presented the calculation up to number of sites $N \simeq 5000$, it is possible to extend the calculation to the larger number of $N = 5000$. But we believe that the essential behaviour of the string solutions is clarified.

In particular, we have studied the properties of the string solutions which are classified into two types, EKS-string and V-string. For the EKS-string, we find clear evidence of the violation of the complex solutions, and at some number N , they become real solutions. We confirm the results up to $N = 417$. Initially, the EKS-string is a usual string solution, that is, the imaginary part of the EKS-string is $1/2$. However, it deviates from $1/2$ when the number of sites N increases, and the imaginary part of the EKS-string becomes zero. On the other hand, the V-string behaves in a rather normal way. We show that the real part and the imaginary part of the V-strings behave as N and \sqrt{N} , respectively, and the calculated results are consistent with the prediction by the $1/N$ expansion method. Finally, the complex solutions of the XXX model in the Bethe ansatz method are classified into three types of solutions for a given N . The first type is given by the string solution based on the string hypothesis. The second is given by the EKS-string whose imaginary part is lower than $1/2$. The third is the V-string which behaves as N^α with $\alpha = 1$ or $1/2$.

The EKS-string and V-string are out of the solutions based on the string hypothesis but *not* out of the Bethe ansatz solutions. Therefore, the number of states which is given by the Bethe ansatz method is unchanged. Further, the number of complex solutions is less than the prediction of the string hypothesis. But, as shown in equations (33) and (34), the difference is of order \sqrt{N} . Therefore, a thermodynamic quantity such as entropy cannot be affected by these phenomena.

The string hypothesis has been applied to many exactly solvable models and has given physically plausible results. However, even for the XXX model, some of the string solutions

break down. Therefore, we must carefully analyse the exactly solvable model in the Bethe ansatz method with the string hypothesis [16, 17]. In the massive Thirring model, the bound state is calculated using the string hypothesis [18]. But the recent investigation shows that it is not correct [19–21]. We will investigate for the future the issue of how these violations of the string solutions affect the bound state problem of the massive Thirring or XYZ models.

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