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LETTER TO THE EDITOR

Analysis of the Bethe-ansatz equations for the anisotropic SU(2) chain

Francisco C Alcaraz†§ and Márcio J Martins†‡||

† Departamento de Física, Universidade Federal de São Carlos, Cxp-676, 13560-São Carlos-SP, Brazil

‡ Instituto de Física e Química de São Carlos, Universidade de São Paulo, Cxp-369, 13560-São Carlos-SP, Brazil

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Abstract. The Bethe-ansatz equations for the anisotropic spin- S Heisenberg chain are analysed numerically. The position of the roots for the whole spectrum is calculated for the spin-1 model in a chain of width $N = 4$. Some states are presented which violate the normally accepted string hypothesis.

According to the theory of quantum integrable systems any solution of the Yang-Baxter equations [1, 2] is related to some one-dimensional spin model. One of these solutions, with U(1) symmetry, corresponds to the generalisation of the anisotropic Heisenberg spin for arbitrary integer or half-integer spin S (XXZ- S model).

The diagonalisation of the XXZ- S model is based on the quantum inverse scattering method [3] which is an algebraic formulation of the original Bethe ansatz [4]. The eigenenergies and momenta of the eigenspectrum are given in terms of the roots $\{\lambda_j\}$ of a system of algebraic equations, the so-called Bethe-ansatz equations (BAE).

From the U(1) symmetry of the XXZ- S model its associated Hilbert space can be separated into disjoint sectors labelled by the eigenvalues $r = 0, 1, 2, \dots$ of the z component of the total spin (U(1) charge). The associated BAE for the sector r of the XXZ- S model in a chain of N sites are

$$\left(\frac{\sinh \gamma(\lambda_j - iS)}{\sinh \gamma(\lambda_j + iS)}\right)^N = \prod_{\substack{k=1 \\ k \neq j}}^{SN-r} \frac{\sinh \gamma(\lambda_j - \lambda_k - i)}{\sinh \gamma(\lambda_j - \lambda_k + i)} \quad j = 1, 2, \dots, SN-r \quad (1)$$

where γ is the parameter of anisotropy. The energy and momentum, for a given distribution of the roots $\{\lambda_j\}$, are given by

$$E = \frac{\sin^2(2S\gamma)}{2S} \sum_{j=1}^{NS-r} \frac{1}{\cos(2S\gamma) - \cosh(2\lambda_j)} \quad (2)$$

and

$$P = \sum_{j=1}^{NS-r} 2 \tan^{-1}[\coth(S\gamma) \tan \lambda_j] \quad (\text{mod } 2\pi) \quad (3)$$

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respectively. Some properties in the infinite-size limit have been considered [5, 6]. In this limit the solution of the BAE is based on the string hypothesis, which claims that the zeros corresponding to any solution of (1) cluster in a series of strings of the form [5]

$$\lambda_j^{n,\alpha} = \lambda_j^n + i(n+1-2\alpha)/2 \quad \alpha = 1, 2, \dots, n \quad (4)$$

where λ_j^n (real) and n (non-negative integer) are the centre and size of the string. Assuming (4) we can parametrise an arbitrary configuration of zeros, in the sector r , by giving the number ν_n of strings of size n such that $\sum_n n\nu_n = NS - r$. However, deviations from the string hypothesis for excited states have been found [7, 8]. In this letter we consider the deviations from the string picture by solving (1) numerically for spin $S \geq 1$ and finite chain N .

In order to see the possible structure of zeros of the BAE it is an instructive exercise to solve initially these equations for small chains. In the case of $S = 1$ and $N = 4$, the possible configurations of zeros are shown in table 1. In figure 1 and table 1(a) we introduce our notation for the distribution of the zeros. Table 1(a) give us the exact location of the BAE roots for some eigenstates and exemplifies the excitations shown, in a schematic form in figure 1. In table 1(b) we present for all sectors a complete picture of zeros for all the eigenstates. We also show in table 1 their corresponding energies and momenta in order to give us a complete idea of the whole spectrum. We observe from these tables that when a root with imaginary part $(\pm\pi/2\gamma)$ (roots of type A_k^\pm in figure 1, which are represented by the symbol $*$) is added to a configuration of the sector r ($r > 0$) it produces a configuration of the sector $r-1$. For example, the state with three zeros located at $(0, +ia - ia)$, in the sector $r = 1$, like the configuration $1_0 2_0$ in table 1, goes to the state with four zeros located at $(i\pi/2\gamma, 0, ib, -ib)$ in the sector $r = 0$, like the configuration $(1_0 A_0^+ 2_0)$ in table 1. Another example is the state with two real zeros $(a, -a)$ in the sector $r = 2$ (configuration 2_0 in table 1(b)) which goes to the state in the sector $r = 1$ with zeros $(i\pi/2\gamma, b, -b)$ (configuration $2_0 A_0^+$ in table 1(b)) or to the state, in the sector $r = 0$, with zeros $(a' + i\pi/2\gamma, -a' - i\pi/2\gamma, b', -b')$ (configuration $A_{-2}^- 2_0 A_2^+$). Moreover our numerical solutions of the BAE, up to lattices of size $N = 40$ and for spin $S = 1, 3/2$ and 2 , indicate that the zeros for type A_k^\pm have the imaginary part always fixed at the value $(\pm\pi/2\gamma)$, independently of the lattice size and the spin S . These types of zeros do not fit the string assumption (4) but can be included in a more general formulation of this assumption [6]. In the isotropic limit, $\gamma \rightarrow 0$, these zeros go to infinity producing a degeneracy between states of different sectors, because, in this limit, an infinite zero does not contribute to the energy (see equation (2)).

We also verify numerically the appearance of special structures of zeros that, as $N \rightarrow \infty$, go towards a configuration that violates the original string assumption (4) or its extended version [6]. The first structure of this type occurs in the sector $r = 0$ of the spin-1 model. This structure involves four zeros and resembles a 4-string excitation for small N . However, as N increases, the imaginary parts of the two farthest (Y_2) and nearest (Y_1) zeros from the real axis tend toward (2) and $(1/2)$, respectively, in contrast with the 4-string structure (4), where these values are $(3/2)$ and $(1/2)$, respectively. In order to illustrate this defective structure, and compare it with the normal 4-string one, we give in tables 2(a) and (b), for several values of N , the imaginary parts (Y_1) and (Y_2) of the zeros for these structures. The roots shown in table 2 appear together with a sea of $(N-4)/2$ strings of size 2. We observe, however, that, for $N \geq 8$, these 2-string seas, associated with tables 2(a) and (b), have a different

Table 1. (a) The complex roots of the BAE and momenta for some states, in the sector $r=0, 1, 2$ and 3 , of the spin model with coupling $\gamma = \pi/10$ and chain size $N=4$. The symbols in the first column characterise the distribution of roots (see also figure 1). (b) The distribution of zeros of the BAE, energies and momenta for the complete set of states for the spin-1 model with coupling $\gamma = \pi/10$ and chain size $N=4$. The symbols in the first column characterise the distribution of zeros (see also figure 1). The energies with the superscript * are doubly degenerate; the configuration of zeros corresponding to the other state is obtained by changing the sign of the real part of the zeros.

(a)

| $\{\nu_n\}$ | r | P | $\{\lambda_j\}$ |
|--------------------------|-----|---------|---|
| $2_{1/2}2_{-1/2}$ | 0 | 0 | $\pm 0.295\ 7747 \pm 0.551\ 2269i$ |
| $A_0^+1_02_0$ | 0 | 0 | $5i, 0, \pm 0.451\ 9395i$ |
| $A_{-2}^-1_{-1}1_1A_2^+$ | 0 | 0 | $1.972\ 2917 + 5i, -1.972\ 217 - 5i, \pm 0.713\ 8511$ |
| 1_02_0 | 1 | π | $0, \pm 0.444\ 7932i$ |
| 1_{-1} | 3 | π | $-1.073\ 1427$ |
| $A_{1/2}^+1_1$ | 2 | $\pi/2$ | $0.310\ 2752 + 5i, 1.002\ 8587$ |

(b)

| r | $\{\nu_n\}$ | E/N | P | r | $\{\nu_n\}$ | E/N | P |
|-----|----------------------------------|--------------|---------|-----|----------------------------|--------------|---------|
| 0 | $2_{1/2}2_{-1/2}$ | -0.986 4962 | 0 | 1 | $2_{-1/2}A_1^+$ | -0.432 8636* | $\pi/2$ |
| 0 | $1_0A_0^+2_0$ | -0.774 5026 | π | 1 | 3_0 | -0.327 2542 | 0 |
| 0 | $A_{-2}^-2_0A_2^+$ | -0.585 8934 | 0 | 1 | $1_{-1/2}A_0^+1_{1/2}$ | -0.266 7634 | 0 |
| 0 | 1_03_0 | -0.553 3813 | π | 1 | $3_{1/2}$ | -0.244 3134* | $\pi/2$ |
| 0 | $1_{-1/2}2_{1/2}A_1^+$ | -0.509 4177* | $\pi/2$ | 1 | $2_{-1}A_{1/2}^+$ | -0.202 2542* | π |
| 0 | $2_{-1/2}A_1^-A_{-2}^-$ | -0.428 3813* | $\pi/2$ | 1 | $A_{-3/2}^-1_0A_{3/2}^+$ | -0.188 0810 | π |
| 0 | $3_0A_0^+$ | -0.303 3813 | 0 | 1 | $A_{-2}^-1_1A_1^+$ | -0.075 6080* | $\pi/2$ |
| 0 | $A_{-2}^-1_{-1/2}1_{1/2}A_2^+$ | -0.262 2929 | 0 | 1 | $A_{-5/2}^-A_0^+A_{5/2}^+$ | +0.051 0924 | 0 |
| 0 | $3_1A_2^+$ | -0.251 1805* | $\pi/2$ | 2 | 2_0 | -0.618 1531 | 0 |
| 0 | 4_0 | -0.236 7097 | 0 | 2 | $2_{-1/2}$ | -0.444 1201* | $\pi/2$ |
| 0 | $2_{-1}A_{-1}^+A_2^+$ | -0.202 2542* | π | 2 | $1_{-1}1_1$ | -0.279 5084 | 0 |
| 0 | $A_{-3}^-1_0A_0^+A_3^+$ | -0.183 3872 | π | 2 | $A_0^+1_0$ | -0.202 2542 | π |
| | | | | 2 | 2_1 | -0.202 2542* | $\pi/2$ |
| 0 | $A_{-3}^-A_{-1/2}^-A_{7/2}^+1_1$ | -0.072 2916* | $\pi/2$ | 2 | $A_{1/2}^+1_1$ | -0.085 3883* | $\pi/2$ |
| 0 | $A_{-4}^-A_{-1}^-A_1^+A_4^+$ | +0.054 4854 | 0 | 2 | $A_{-1}^-A_1^+$ | +0.040 8989 | 0 |
| 1 | 2_01_0 | -0.793 6816 | π | 3 | 1_0 | -0.226 1271 | π |
| 1 | $A_0^+2_0$ | -0.593 3460 | 0 | 3 | 1_{-1} | -0.101 1271* | $\pi/2$ |
| 1 | $1_{-1/2}2_{1/2}$ | -0.508 4864* | $\pi/2$ | 3 | A_0^+ | +0.023 8728 | 0 |

size dependence. The 2-string sea associated with table 2(a) (table 2(b)) always has its zeros with imaginary part having an absolute value bigger (smaller) than $1/2$.

Our numerical analysis for spin $S=3/2$ and $S=2$ also indicates another type of zero structure which violates the string assumption. In fact we believe that this structure exists for all $S \geq 3/2$. In order to explain these structures let us restrict ourselves to lattice size multiples of 4. For these chains, according to the string hypothesis, the state with lowest energy in the sector $r=1$ is formed by $(N/2-2)$ strings, of size $2S$, symmetrically distributed with respect to the imaginary axis, and two strings of size $2S$ and $(2S-1)$ located at the imaginary axis. However, the solution of the BAE, for finite N , shows that the $(4S-1)$ pure imaginary zeros, instead of forming the strings of size $2S$ and $2S-1$, prefer to form a complex structure where the four farthest zeros, from the real axis, are located at the corners $(\lambda_R \pm i\lambda_I)$ of a rectangle with the remaining zeros forming, along the imaginary axis, one string of size $(2S-2)$ and another of size

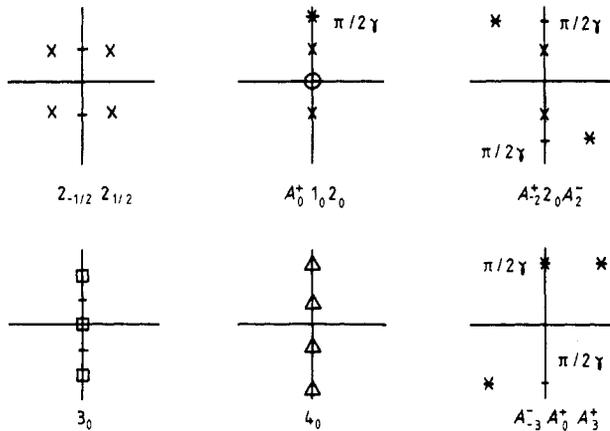


Figure 1. Some typical configurations of the complex zeros of the BAE, for the spin-1 model, in an $N=4$ sites chain. The vertical (horizontal) axis represents the imaginary (real) part of the roots. The symbols B_k with $B=1, 2, 3, 4$ or A^\pm denote strings of size 1, 2, 3, 4 or an excitation with an imaginary part ($\pm\pi/2\gamma$), respectively. The subscript k is the nearest integer or half-integer which better represents the real part of the zeros forming the excitation. The strings of size 1, 2, 3 and 4 are represented by circles (\circ), crosses (\times), squares (\square) and triangles (\triangle) while the excitations of type A are represented by asterisks ($*$).

Table 2. The location, for several values of lattice size N , of the zeros of the BAE which resemble a 4-string structure, for the spin-1 model with anisotropy $\gamma = \pi/6$. The imaginary parts of the two nearest and farthest zeros are ($\pm Y_1$) and ($\pm Y_2$). As N increases, the zeros tend toward a defective structure in (a) and to the string of size 4 in (b) (see text). The eigenenergies corresponding to the distribution of roots where the above structures occur are also shown.

(a)

| N | E/N | Y_1 | Y_2 |
|-------|-------------|------------|------------|
| 8 | -0.573 8621 | 0.502 5052 | 1.577 2115 |
| 16 | -0.704 6703 | 0.503 4479 | 1.657 8458 |
| 24 | -0.729 9104 | 0.503 0303 | 1.706 1569 |
| 32 | -0.738 7478 | 0.502 5694 | 1.738 6620 |
| 40 | -0.742 8242 | 0.502 1985 | 1.762 3723 |
| Extr. | -0.750 (1) | 0.500 (1) | 1.99 (1) |
| Conj. | -0.75 | 0.5 | 2 |

(b)

| N | E/N | Y_1 | Y_2 |
|-------|-------------|--------------|------------|
| 8 | -0.419 6783 | 0.500 0400 | 1.506 5420 |
| 16 | -0.582 4816 | 0.500 0038 | 1.502 0327 |
| 24 | -0.638 7408 | 0.500 0017 | 1.500 9875 |
| 32 | -0.666 8884 | 0.500 0003 | 1.500 5840 |
| Extr. | -0.750 (4) | 0.500 00 (2) | 1.4999 (8) |
| Conj. | -0.75 | 0.5 | 1.5 |

($2S-3$). In figure 2(a) we draw this complex structure of zeros for the spin-2 model. As N increases the real parts (λ_R) of the zeros forming the rectangle decrease while the imaginary parts (λ_I) tend toward $i(S-1/2)$. Consequently, in the $N \rightarrow \infty$ limit, the complete structure of roots for the eigenvector is composed by $(N/2-2)$ strings of size $2S$, two other strings of size $(2S-2)$ and $(2S-3)$ and a pair of roots located at $\pm i(S-1/2)$, in contradiction to the string assumption. In table 3 we show, for $S=3/2$ and $S=2$, the tendency to form this defective pair of zeros by giving, for lattice size up to $N=40$, the values of λ_R and λ_I . This defective structure has been realised before [8, 9] in the special case where $\gamma=0$. More generally, from our numerical results we conjecture, for $S \geq 3/2$, that defective structures, of the kind described above, will also occur in other sectors $r \neq 1$ of the associated Hilbert space. More precisely they will appear in the configuration of zeros which corresponds to the lowest eigenenergy of the set of sectors $r=1+2Sj$, where $j=0, 1, 2, \dots$. According to the string hypothesis the configuration of zeros expected for such states is formed by $\nu_{2S}=(N/2-j-1)$ strings of size $2S$ and a single string of size $(2S-1)$. If j is even the same structure, described previously for the sector $r=1$, occurs, *mutatis mutandis*. However, if j is odd, the $(2S-1)$ zeros which would form, according to the string hypothesis, a pure imaginary string of size $(2S-1)$, prefer to remain in the imaginary axis but, as N

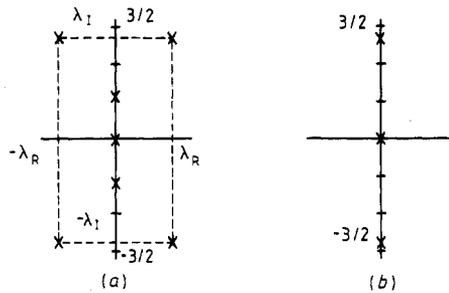


Figure 2. Some configurations of roots of the BAE, for the spin-2 model, which deviate from the string hypothesis (see the text). The crosses (x) represent the roots and the horizontal (vertical) axis their real (imaginary) part. Configuration (a) ((b)) appears in the distribution of roots which gives the lowest energy of sectors $r=1, 9, 17, \dots$ ($r=5, 13, 21, \dots$).

Table 3. The location, for several lattice sizes N , of the outermost zeros of the BAE, ($\lambda = \lambda_R \pm i\lambda_I$), for some excitations which deviate from the string hypothesis. The excitations appearing in the sector $r=1$ of the spin $S=3/2$ and $S=2$ model (sector $r=4$ of the spin $S=3/2$ model) are of the type shown in figure 2(a) (figure 2(b)).

| N | $S=3/2, r=1$ | | $S=2, r=1$ | | $S=3/2, r=4$ |
|-------|--------------|-------------|-------------|-------------|--------------|
| | λ_R | λ_I | λ_R | λ_I | λ_I |
| 8 | 0.108 7111 | 0.928 5499 | 0.122 9136 | 1.471 8195 | 0.605 9265 |
| 16 | 0.060 6575 | 0.973 7695 | 0.062 2109 | 1.490 7608 | 0.674 6341 |
| 24 | 0.041 1062 | 0.984 9942 | 0.041 5598 | 1.494 9970 | 0.733 8721 |
| 32 | 0.031 0002 | 0.989 7428 | 0.031 1958 | 1.496 7277 | 0.787 1811 |
| 40 | 0.024 8642 | 0.992 3047 | 0.024 9678 | 1.497 6352 | 0.836 7649 |
| Extr. | 0.000 1 (4) | 1.000 0 (8) | 0.000 3 (1) | 1.499 8 (1) | 1.0 (2) |
| Conj. | 0 | 1 | 0 | 1.5 | 1 |

increases, tend toward the structure composed by one string of size $(2S-3)$ and a defective pair of zeros located at $\pm i\lambda_1 = \pm i(S-1/2)$. In figure 2(b) we draw this structure, in the case of $S=2$ and $r=5$. In table 3 we also show the corresponding location, for some lattice sizes, of the pure imaginary defective pair, in the case $S=3/2$ and $r=4$. These defective structures will also appear in excited states of the other sectors. They will occur because, as already discussed, if we add to them excitations which have a pure imaginary part $(\pm\pi/2\gamma)$ (type A_k^\pm in figure 1), we obtain a configuration of zeros which describes excited states of different sectors.

As a last remark we mention that these defective excitations may, in principle, produce a different dispersion relation, in the infinite-size limit, from that calculated originally by Sogo [5] based on the string hypothesis. However, after some lengthy calculation, in which these defective structures are included, we can show that this dispersion relation remains the same.

In conclusion, the numerical analysis of the BAE for the $XXZ-S$ model shows that the normally accepted string hypothesis does not provide a very accurate description of the structure of roots for these equations.

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