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New solutions of the Bethe ansatz equations for the isotropic and anisotropic spin-$\frac{1}{2}$ Heisenberg chain

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Abstract. Bethe ansatz equations (BAE) are investigated for the isotropic spin-$\frac{1}{2}$ Heisenberg chain as well as the XXZ chain with real solutions characterized by identical integers in the logarithmic form of the BAE. Such states do not belong to the usual classification scheme (string hypothesis). They always exist in critical sectors with respect to the total spin of the chain and the anisotropy.The conception of holes has to be changed in this case, because there occur more holes than expected. The finite-size corrections for the XXX model are calculated including complex roots and the new type of real solutions with repeating integers. The 'tower structure' predicted by the hypothesis of conformal invariance is shown to remain unchanged.

1. Introduction

The Heisenberg model represents a quantum-mechanical generalization of the Ising model which describes the spin interaction of a system. Its solution is given by the familiar Bethe ansatz equations (BAE) (Bethe 1931) related to the Yang–Baxter algebra, quantum groups and statistical physics.

In this paper we investigate the one-dimensional spin chain with nearest-neighbour interaction and periodic boundary condition ($N+1 \equiv 1$). The isotropic Hamiltonian (XXX model) in the antiferromagnetic case ($J > 0$) can be given by a sum of Pauli matrices having the form

$$H = \frac{J}{4}\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z - 1) \tag{1}$$

that is the limit ($\gamma \to 0$) of the anisotropic XXZ model

$$H = \frac{J}{4}\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \cos\gamma\,\sigma_i^z\sigma_{i+1}^z). \tag{2}$$

The solutions have to satisfy the Bethe ansatz equations

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}}\right)^N = \prod_{\substack{k=1\\k\neq j}}^{r}\frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i} \qquad j = 1\ldots r \tag{3}$$

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where the parameters λ_j—often referred to as rapidities or roots—determine all the other interesting quantities as for instance the energy

$$E = -\frac{J}{2}\sum_{k=1}^{r}\frac{1}{\lambda_k^2+\frac{1}{4}} \tag{4}$$

or the momentum

$$P = \frac{1}{i}\sum_{k=1}^{r}\ln\frac{\lambda_k+\frac{i}{2}}{\lambda_k-\frac{i}{2}} \tag{5}$$

of the chain (see e.g. Faddeev and Takhtajan 1981).

For large N one assumes the so-called string hypothesis (Takahashi 1971) which claims that any solution consists of a series of strings in the form

$$\lambda = x + \mathrm{i}\left(\frac{n+1}{2} - m\right) \qquad m = 1\ldots n \qquad x\ldots\text{real}. \tag{6}$$

It is useful to take the logarithm of the algebraic BAE (3)

$$\frac{Q_k}{N} = \frac{1}{\pi}\tan^{-1}(2\lambda_k) - \frac{1}{N}\sum_{l=1}^{r}\frac{1}{\pi}\tan^{-1}(\lambda_k - \lambda_l). \tag{7}$$

Because of the logarithmic branches either a set of integers or a set of half-integers occurs which depends on N and r

$$Q_k = \frac{N-r+1}{2} - k \qquad k = 1, 2, \ldots\,. \tag{8}$$

A general assumption in the string hypothesis is a one-to-one correspondence between a rapidity λ_k and a number Q_k, i.e. strings with the same length n should *not* have the same integers in order to count the total number of configurations by the set $\{Q_k\}$. Despite the fact that there are a lot of investigations about the BAE, Vladimirov (1984) and Eßler *et al* (1991, 1992) found a new type of real solutions which were overlooked in recent years. Eßler and co-workers analysed the BAE for the two particle sector ($r = 2$) of the XXX model. New pairs of unexpected, real solutions are found to develop where the corresponding integers of the BAE are identical, although their rapidities are different. Such two additional roots can appear, if the lattice length N is greater than a critical value $N = 21.86$. Furthermore, it was shown by graphical methods (Essler *et al* 1991, 1992) that this new case is connected with a loss of complex roots. Thus, the total number of solutions (2^N) remains unchanged—in agreement with the assumption that all eigenstates can be given by the $SU(2)$ extended Bethe ansatz (Faddeev and Takthajan 1981). But a crucially new type of real solutions is obtained, which is not describable by the string hypothesis. Due to the disappearence of complex roots, the pairs of real roots characterized by repeating integers may be considered as degenerate complex strings.

In comparison to the ground state, the two-particle sector with $N \geqslant 22$ (where the new solutions occur) belongs to the ferromagnetic sector. The normal, 'undegenerate' ground state is determined by $r = 11$ magnons for the minimal critical lattice length $N = 22$. Therefore, the first motivation of this paper consists in a consideration of such states in the antiferromagnetic sector having more than two magnons. An analytical or graphical investigation of the BAE for calculating *all* possible solutions leads to several complications for $r > 2$ or a higher number of roots. We consider only the simple real case without any complex root if not stated otherwise. Indeed, we have found such a kind of real solutions for *every* number of rapidities by means of numerical iterations. They can exist in a region characterized by the antiferromagnetic sector. This will be described in sections 2, 3 and 4.

On the other hand, the new type of roots should be allowed for in the so-called finite-size corrections related to critical phenomena of 2D systems with second-order phase transitions. Critical systems are assumed to have a conformally invariant behaviour. According to this hypothesis Cardy (1984, 1987) made predictions about the spectrum (conformal towers) of the corresponding 1D quantum systems by a comparison between a finite strip and a planar infinite system (with the ground-state energy $E_\infty = AN$),

$$E_0 = AN - \frac{\pi}{6N}c \tag{9}$$

$$E - E_0 = \frac{2\pi}{N}(x + m + \bar{m}) \tag{10}$$

$$P - P_0 = \frac{2\pi}{N}(l + m - \bar{m}) \tag{11}$$

where x, l are the scaling indices, m and $\bar{m}$ are non-negative integers and c is the conformal charge. The correlation length is known to be infinite in a critical system. It is directly proportional to the inverse of the gap $E - E_0$, which therefore has to tend to zero for $N \to \infty$. A reverse test is possible by a comparison of the computed excitations of a solvable model. In section 5 we calculate the excitation spectrum of the isotropic Heisenberg chain. Rapidities with repeating integers are included.

2. Characterization of real solutions for the isotropic chain

Using the BAE (7) we can introduce the following function

$$z(\lambda) = \frac{1}{\pi}\tan^{-1}(2\lambda) - \frac{1}{N}\sum_{l=1}^{r}\frac{1}{\pi}\tan^{-1}(\lambda - \lambda_l) \tag{12}$$

where the roots λ_l in the sum are assumed to be known. Then any root λ_k is determined by a (half-)integer Q_k:

$$Q_k = Nz(\lambda_k). \tag{13}$$

That means that the set of numbers $\{Q_{\text{root}}\}$ fixes all roots $\{\lambda_{\text{root}}\}$. But in the general case we obtain more real solutions. A hole λ_{hole} is a solution with a number Q_{h}

$$Q_{\text{h}} = Nz(\lambda_{\text{hole}}) \tag{14}$$

which differs from all roots $\lambda_{\text{hole}} \notin \{\lambda_{\text{root}}\}$. Notice that only roots are summed up in (12). Holes do not occur in the original algebraic form (3) of the BAE and they have no direct relevance. Due to the asymptotic behaviour of $z(\lambda)$,

$$Nz(\pm\infty) = \pm\frac{N-r}{2} \tag{15}$$

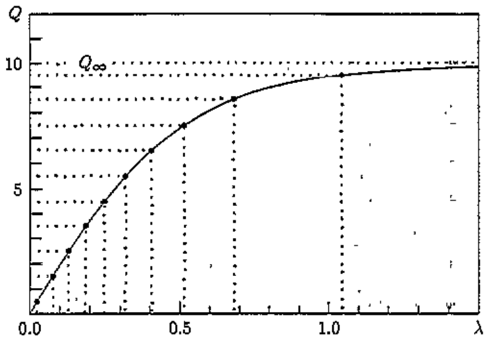

Figure 1. Behaviour of $Nz(\lambda)$ for the ground state, $\lambda > 0$, $N = 40, r = 20$; full circles: roots.

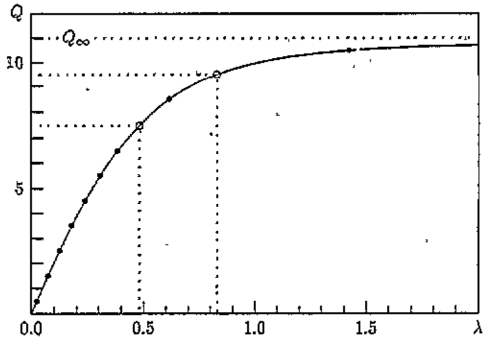

Figure 2. Behaviour of $Nz(\lambda)$ for a symmetrical state with four holes, $\lambda > 0$, $N = 40, r = 18$; full circles: roots, open circles: holes.

it is supposed that the choice of Q_k is restricted by maximal and minimal values

$$Q_{\max} = Nz(\infty) - \tfrac{1}{2} = \frac{N-r-1}{2} \qquad Q_{\min} = -Q_{\max}. \tag{16}$$

($Nz(\infty)$ is a half-integer if the Q_k have to be integers, and vice versa, so that we must add $-\frac{1}{2}$.) The ground state ($r = N/2$) is known to be characterized by real roots only. No hole appears in the set of roots. According to (16) we can write

$$Q_{\max} = \frac{N}{4} - \frac{1}{2} \tag{17}$$

and the total number I of all Q_k within the interval $[Q_{\min}, Q_{\max}]$ is

$$I = Q_{\max} - Q_{\min} + 1 = N/2. \tag{18}$$

Therefore, any root must correspond to a number Q_k. The correspondence is easy to see in figure 1 calculated by the exact (numerical) solutions. The function $z(\lambda)$ determining this relation between λ_k and Q_k is also monotone for the lowest excitations ($r < N/2$) (cf figure 2). Here the normal case is assumed with non-repeating integers. The maximum $Q_{\max}$ increases (16) so that *two* holes are found if one root is dropped (the number of roots r decreases by one). This behaviour is often referred to as the backflow effect. According to the assumed one-to-one correspondence, the number of all real solutions is equal to the number of integers

$$r + h = Q_{\max} - Q_{\min} + 1 = N - r$$

and the total number of holes per configuration reads

$$h = N - 2r. \tag{19}$$

Since the choice of Q_{hole} is free within the interval $[Q_{\min}, Q_{\max}]$, we obtain two degrees of freedom by dropping one root.

We solved the BAE by numerical iterations

$$\lambda_k^{(n+1)} = \frac{1}{2}\tan\left(\frac{\pi Q_k}{N} + \frac{1}{N}\sum_{j=1}^{r}\tan^{-1}(\lambda_k^{(n)} - \lambda_j^{(n)})\right) \tag{20}$$

which are determined by the choice of integers Q_k. In our investigation the series $\{\lambda_k^{(0)}, \lambda_k^{(1)}, \lambda_k^{(2)}, \ldots\}$ is found to be convergent ($n \to \infty$) for all arbitrarily chosen configurations $\{Q_k\}$. The starting values $\{\lambda_k^{(0)}\}$ were non-critical: the iterations given by the same quantities N, r and $\{Q_k\}$ converged to the same solution for any $\lambda_k^{(0)}$. But a starting root $\lambda_k^{(0)}$ has to be different from any other value $\lambda_n^{(0)}$ in order to include the later consideration of degenerate states with repeating integers. At first we calculate the ground state with a lattice length $N > 22$ (e.g. $N = 40$, $r = 20$). Now, step by step, a root was dropped. The set $\{Q_k\}$ was changed within $[Q_{\min}, Q_{\max}]$ and all possible states with *non-repeating* integers describing the real roots were computed. Because of the smooth behaviour of $z(\lambda)$ one always obtains a convergent solution. Furthermore, a description by roots only is complete since the position of holes is read off from $z(\lambda)$ (cf figure 2). In the normal case the resulting integers of *holes* differ from integers of any other hole *and* root. The function $z(\lambda)$ remains monotone. However, the behaviour of z begins to change below a certain number of roots r (N is fixed). This function can oscillate in the vicinity of the maximal or minimal root $\lambda_{\max/\min}$ if its corresponding integer is equal to $Q_{\max}$ or $Q_{\min}$, respectively. Although we have a *non-repeating* set of roots, we obtain two different, finite holes $\lambda_{h_1} \neq \lambda_{h_2}$ with the same integers $Q_{h_1} = Q_{h_2} = Q_{\max}$. This situation is shown in figure 3. Now one can try to exchange such a hole (we call it 'virtual hole') by a root. Below a critical r, which is in general slightly smaller than the value described above, a state is possible with two *finite* roots (a double root) and one virtual hole $\lambda_{r_1} \neq \lambda_{r_2} \neq \lambda_h$ having identical integers at $Q_{\max} = Q_{r_1} = Q_{r_2} = Q_h$ (see figure 4). If more roots are dropped, one can also construct configurations where four or more integers are equal (figure 5). There are even solutions with repeating integers smaller than $Q_{\max}$ (cf figure 6). In principle, all imaginable degenerate states seem to be possible that have an arbitrary choice of integers for *the roots*—repeating or non-repeating on the edge—with no regard for the accompanying holes. The existence of such a configuration should depend on a relation between the lattice length N and the number of magnons r. One can introduce a critical value for r being a function of N and the set $\{Q_k\}$

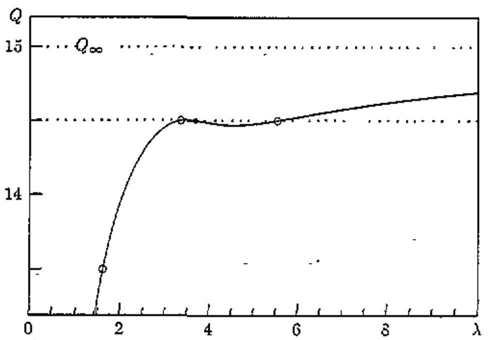

Figure 3. Degenerate behaviour of $Nz(\lambda)$ on the edge for a symmetrical state with virtual holes at $Q_{\max} = 14.5$, $\lambda > 0$, $N = 40$, $r = 10$; full circles: roots, open circles: holes.

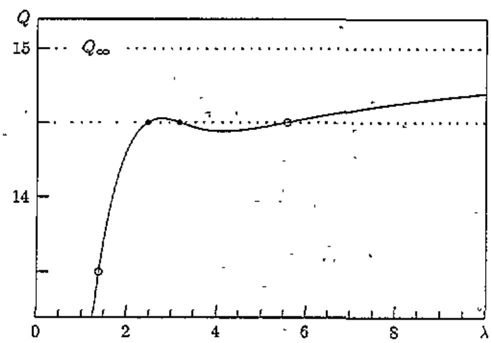

Figure 4. Behaviour of $Nz(\lambda)$ on the edge for a symmetrical state with a double root at $Q_{\max} = 14.5$, $\lambda > 0$, $N = 40$, $r = 10$; full circles: roots, open circles: holes.

$$r \leqslant r_{\text{crit}} = r_{\text{crit}}(N, \{Q_k\})$$

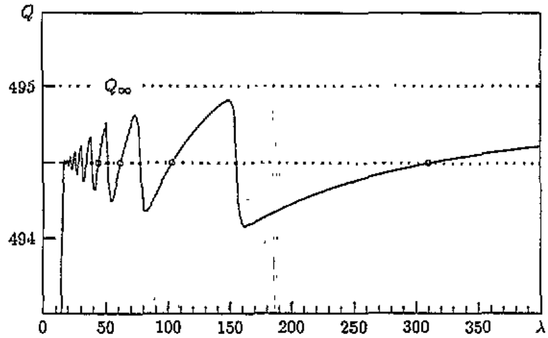

Figure 5. Behaviour of $Nz(\lambda)$ for a state with 10 roots and nine virtual holes at $Q_{max} = 494.5$, $\lambda > 0$, $N = 1000$, $r = 10$; full circles: roots, open circles: holes.

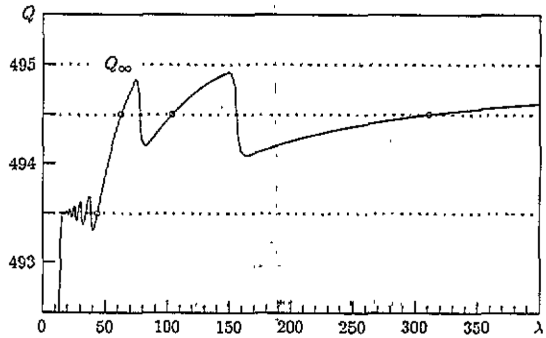

Figure 6. Behaviour of $Nz(\lambda)$ for a state with two roots (three virtual holes) at $Q_{max} = 494.5$ and eight roots (seven virtual holes) at $Q_{max} - 1 = 493.5$, $\lambda > 0$, $N = 1000$, $r = 10$; full circles: roots, open circles: holes.

or vice versa

$$N \geqslant N_{crit} = N_{crit}(r, \{Q_k\}). \tag{21}$$

3. Lowest 'degenerate' excitations

The excitations of the Heisenberg chain are described by the total spin

$$S = \frac{N}{2} - r \tag{22}$$

and by the position of the integers Q_k in the set. For the lowest excitations the holes Q_h must lie on the edge of the interval $[Q_{min}, Q_{max}]$. Since we are interested in 'degenerate' states (i.e. configurations with repeating integers) in the antiferromagnetic sector, we are looking for such states in the vicinity of the ground state ($S = 0$). The following symmetrical arrangement was considered with repeating integers for two roots (a double root)

$$Q_1 = Q_2 = -Q_r = -Q_{r-1} = \frac{N - r + 1}{2} - \kappa \quad \kappa = 1, 2, \ldots \tag{23}$$

and non-repeating integers for the remaining numbers

$$Q_3 = \frac{r-1}{2} - 2 \qquad Q_4 = \frac{r-1}{2} - 3, \ldots \quad Q_{r-2} = -\frac{r-1}{2} + 2 \tag{24}$$

(N is always even). The solutions are calculated for $r = 4, 6, 8, \ldots$ where the two interesting roots λ_1 and λ_2 tend to different rapidities ($\lambda_1 \neq \lambda_2$). This is possible above a critical lattice length N_{crit}, and if $\lambda_1^0 \neq \lambda_2^0$ (by virtue of (20)). Below N_{crit} the parameters λ_1 and λ_2 always converge to the same value that must be excluded because of the 'Pauli principle for *spectral parameters* λ'. The relation between the critical length and r is listed in table 1.

Table 1. Critical lattice length N_{crit} for configurations with a double root at $Q_{\max}$ (XXX chain).

r	N_{crit}	S	r	N_{crit}	S
10	38	9	400	820	10
30	78	9	600	1222	11
40	100	10	800	1622	11
50	120	10	1000	2022	11
100	220	10	2000	4022	11
200	420	10			

A nearly linear correspondence can be seen between N and r. According to $S = N/2 - r$, one can change the interpretation: 'degenerate' solutions are observed above a critical spin $S \geqslant S_{\mathrm{crit}}$, which is a weak function of N. For small lattice length we obtain (cf table 1)

$$S_{\mathrm{crit}} = 9 \qquad \kappa = 1$$

which corresponds to the special case $r = 2$ found by Eßler *et al* ($N_{\mathrm{crit}} = 22 \rightarrow S = N/2 - 2 = 9$). Of course, the numerical results are quite empirical, but above this border states *always* occur that have repeating integers with respect to the BAE of the XXX chain. It follows from our results that the minimal 'degenerate' excitation is closely related to $\kappa = 1$ i.e. $Q_\kappa = Q_{\max}$. If two roots are fixed at $Q_{\max}$ and the position of the remaining numbers Q_k is changed, the critical spin is changed by one in the most extreme case. Real solutions with repeating integers only appear, if one or two *roots* correspond to $\pm Q_{\max}$. All remaining roots and holes have non-repeating integers Q_k with $Q_{\min} < Q_k < Q_{\max}$. If neither a root at $Q_{\min}$ nor at $Q_{\max}$ was choosen, we observed the normal, monotone behaviour of $z(\lambda)$. Nevertheless, states are found to have identical integers at $Q_k < Q_{\max}$ i.e. $\kappa > 1$. But the lattice length (and therefore the excitation) must be much higher for a given r. For further convenience we call them second and higher critical conditions.

We underline that the number of real roots *and* (virtual) holes at the same $Q_k < Nz(\infty)$ must be always odd due to the limit of $z(\lambda \rightarrow \infty)$. Therefore, above a certain lattice length *one root and two holes* were found or *two roots and one hole* appeared by a replacement of some inner root to $Q_{\max}$. (States with three roots belong to a higher critical region, where more virtual holes develop.) In the two cases the total number of holes is greater than the expected value given by (19):

$$h = N - 2r + 2.$$

But the number of holes varies, although N and r are fixed. Namely, if a root corresponds to $Q_{\min}$, one obtains two further virtual holes at $Q_{\min}$

$$h = N - 2r + 4.$$

If no root is fixed at $Q_{\min}$ or $Q_{\max}$, no virtual hole appears in the first critical region:

$$h = N - 2r.$$

Thus, the usual description of the spin S by holes ($S = h/2$) becomes unsuitable. We notice that the number of virtual holes is determined by the set of quantum numbers Q_k. They are always connected with a root on the edge: in this respect a virtual hole has no degrees of freedom.

Excitations lying in the antiferromagnetic part of the spectrum are characterized by the magnetization $\sigma = 2S/N$. Therefore, the behaviour of S_{crit} in the thermodynamical limit $N \to \infty$ is essential for the existence of 'degenerate' solutions at zero magnetization. Our numerical results base on lattice length up to $N = 4000$. (The iteration time increases nearly as N^2.) But unfortunately one cannot yet decide (see table 1) if S_{crit} converges for $N \to \infty$. However, for a finite system there should always occur finite 'degenerate' configurations with respect to S. Also, there are indications that S_{crit} remains finite also in the thermodynamical limit. This will be discussed in the next section by means of the XXZ model.

4. 'Degenerate' solutions in the XXZ case

The logarithmic Bethe ansatz equations for the anisotropic XXZ Hamiltonian (2) read

$$\frac{Q_k}{N} = z(\nu_k) = \frac{1}{2\pi}\Phi(\nu_k, \gamma/2) - \frac{1}{2\pi N}\sum_{m=1}^{r}\Phi(\nu_k - \nu_m, \gamma) \tag{25}$$

$$\Phi(\nu, \gamma) = 2\tan^{-1}(\cot\gamma \tanh\nu). \tag{26}$$

The quantum numbers have the same form as for the isotropic chain (8); one should expect a similar picture for roots with identical integers. The isotropic model is assumed to possess quantum numbers Q_k *with the restriction* $|Q_k| < Q_\infty = Nz(\infty)$ following from (16). Woynarovich (1987b) pointed out that for the XXZ model configurations exist where the largest root lies above Q_∞. In contrast to the BAE of the XXX model, the asymptotic value Q_∞ is a function of a further quantity (2)—the anisotropy γ:

$$Q_\infty = Nz(\infty) = \frac{N-r}{2} - \left(\frac{N}{2} - r\right)\frac{\gamma}{\pi} = \frac{N}{4} + \frac{S}{2} - S\frac{\gamma}{\pi} \tag{27}$$

$$\Phi(\nu \to \infty, \gamma) = \pi - 2\gamma - 2e^{-2\nu}\sin 2\gamma. \tag{28}$$

When γ increases, the asymptotic quantity Q_∞ decreases. Above a certain value of γ/π (which in general is assumed to be a rational number),

$$\frac{\gamma}{\pi} \geqslant \frac{k - \frac{1}{2}}{S} \tag{29}$$

the quantum number $Q_{\max}$ ($k = 1$ according to (8)) may be larger than Q_∞. But the number of real roots and holes at $Q_k > Q_\infty$ *has to be even*. Thus, an additional solution—a virtual hole—appears automatically. *Such a hole must exist for any lattice length.* It is natural to assume that this virtual hole can be exchanged by a root to form a double root. Considering the region $0 \leqslant \gamma < \pi/2$, this is indeed possible for *any* $S \geqslant 2$. We have investigated

Table 2. Ground state ($S = 0$) for $N = 40$ and $p = \pi/\gamma = 5.4$ (XXZ chain).

ν_α	$Q_\alpha = Nz(\nu_\alpha)$
±0.606755901302896583	±9.50000000000000000
±0.396598144013574294	±8.50000000000000178
±0.299655393171647300	±7.50000000000000000
±0.234727721750800117	±6.50000000000000000
±0.184866121411449119	±5.50000000000000000
±0.143529569162347187	±4.50000000000000178
±0.107452328886095738	±3.50000000000000089
±0.074722254955326362	±2.49999999999999911
±0.044073674532395205	±1.49999999999999845
±0.014569363462498965	±0.49999999999999878

numerically the configuration (23), (24) with double roots as a function of κ, S, N and p with

$$p = \frac{\pi}{\gamma}. \tag{30}$$

'Degenerate' solutions with double roots occur in certain sectors (cf figure 7 and tables 2–6) characterized by an upper and lower boundary

$$S_{\text{crit}}^{\max}(p, \kappa) > S_{\text{crit}} > S_{\text{crit}}^{\min}(p, \kappa, N). \tag{31}$$

Table 3. Non-degenerate state $S = 4$ for $N = 40$ and $p = \pi/\gamma = 5.4$ (XXZ chain).

ν_α	$Q_\alpha = Nz(\nu_\alpha)$
±1.82890675122078505	±11.5000000000000018
±0.215047990705406061	±6.49999999999999911
±0.172015337712539129	±5.50000000000000178
±0.134856743277412650	±4.50000000000000000
±0.101598780361121674	±3.50000000000000089
±0.070940275411828319	±2.50000000000000089
±0.041945834664691283	±1.49999999999999822
±0.013882035951251082	±0.50000000000000056

Table 4. Degenerate state $S = 4$ for $N = 40$ and $p = \pi/\gamma = 5.4$ (XXZ chain) with double roots at $Q_\kappa = \pm 11.5$ ($\kappa = 1$).

ν_α	$Q_\alpha = Nz(\nu_\alpha)$
±1.42195906926414151	±11.5000000000000018
±0.985063239227702447	±11.4999999999999982
±0.168080412047442534	±5.50000000000000000
±0.132096913921924575	±4.50000000000000000
±0.0996877772577677568	±3.49999999999999822
±0.0696846493321906513	±2.50000000000000044
±0.0412321201403934370	±1.50000000000000044
±0.0136503725018138049	±0.50000000000000144

Table 5. Degenerate state $S = 4$ for $N = 40$ and $p = \pi/\gamma = 2.502$ (XXZ chain) with double roots at $Q_\kappa = \pm 10.5$ ($\kappa = 2$).

ν_α	$Q_\alpha = Nz(\nu_\alpha)$
±2.77987702595788111	±10.5000000000000000
±2.03213368763034330	±10.5000000000000000
±0.383052118709249378	±5.50000000000000000
±0.299104233659576613	±4.50000000000000089
±0.224746549375348881	±3.50000000000000044
±0.156657638804917620	±2.49999999999999956
±0.0925328158825032415	±1.50000000000000089
±0.0306088102765425078	±0.50000000000000067

Table 6. Degenerate state $S = 10$ for $N = 40$ (XXX chain) with double roots at $Q_\kappa = \pm 14.5$ ($\kappa = 1$).

λ_α	$Q_\alpha = Nz(\lambda_\alpha)$
±3.16367780276306787	±14.5000000000030980
±2.46033396426744799	±14.4999999999970335
±0.108529417879171780	±2.50000000000000266
±0.0644327194673698644	±1.50000000000000133
±0.0213657224561165510	±0.50000000000000044

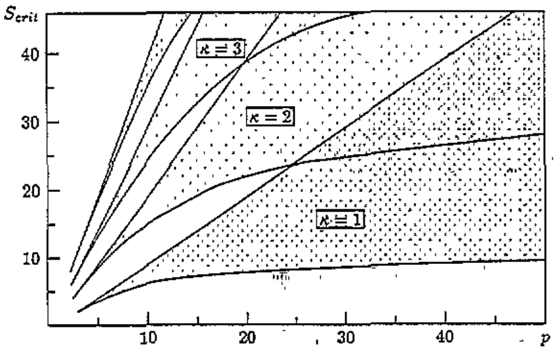

Figure 7. Critical spin sectors (XXZ) for double roots and $\kappa = 1, \ldots, 4$ according to the configuration (23) as a function of $p = \pi/\gamma$ for ($N = 100$).

If the sector κ overlaps with the sector $\kappa + 1$ then double roots are possible both at Q_κ and $Q_{\kappa+1}$. The upper limit

$$S_{\text{crit}}^{\max} = \kappa \cdot p - 1 \tag{32}$$

is a linear function only of p (i.e. γ): this is easy to understand. If we assume a symmetrical state where the largest root at Q_κ is also much larger than all the remaining roots, $\nu_1 \gg \nu_{\beta>1}$, we can split the BAE into two (nearly) independent systems of equations:

$$\frac{Q_\kappa}{N} \simeq \frac{1}{2\pi}\Phi(\nu_1, \gamma/2) - \frac{r-2}{2\pi N}\Phi(\nu_1, \gamma) - \frac{1}{2\pi N}\Phi(2\nu_1, \gamma) \tag{33}$$

$$\frac{Q_\beta}{N} \simeq \frac{1}{2\pi}\Phi(\nu_\beta, \gamma/2) - \frac{1}{2\pi N}\sum_{\alpha=2}^{r-1}\Phi(\nu_\beta - \nu_\alpha, \gamma). \tag{34}$$

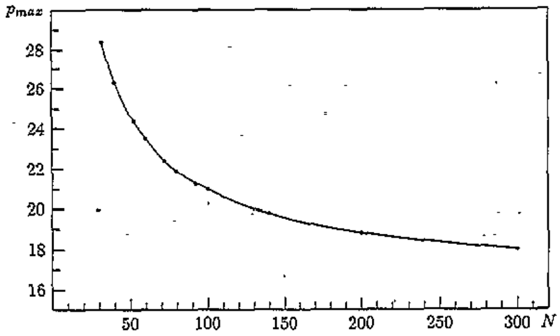

Figure 8. Critical maximum of $p = \pi/\gamma$ for the sector at $S = 8$ and $\kappa = 1$ according to the configuration (23) as a function of N.

Using the asymptotic of (26), we obtain an estimate for the largest root:

$$\nu \sim \frac{1}{2}\ln\frac{N\sin\gamma - (N/2 - S - 2)\sin 2\gamma}{\pi\kappa - (S+1)\gamma}. \tag{35}$$

Now ν_κ tends to infinity for $\gamma \to \pi\kappa/(S+1)$. For $0 < \pi\kappa/(S+1) - \gamma \ll 1$, the largest root is finite but it influences the reduced system (34) only very weakly. This system should obviously possess all non-degenerate configurations, in particular a root with a quantum number at Q_κ. Therefore, the original system having *two* roots at Q_κ becomes degenerate in a natural way with equation (32) as an upper restriction. Decreasing now the spin with respect to (32) at fixed p, the largest root ν_κ decreases too—up to a point where the difference $\nu_{\kappa_1} - \nu_{\kappa_2}$ of the two members of the double root vanishes (lower boundary $S_{\rm crit}^{\rm min}$). One can expand the BAE for $r = 2$ around this critical value $\bar{\nu}$ with $\nu_{\kappa_{1,2}} = \bar{\nu} \pm \delta$:

$$\frac{Q_\kappa}{N} = \frac{1}{2\pi}\Phi(\bar{\nu}, \gamma/2) \tag{36}$$

$$\frac{Q_\kappa}{N} = \frac{1}{2\pi}\Phi(\bar{\nu} \pm \delta, \gamma/2) - \frac{1}{2\pi N}\Phi(\pm 2\delta, \gamma). \tag{37}$$

The condition for $0 < \delta \ll 1$ reads

$$N\left(\cos\gamma + \cos\frac{2\pi Q_\kappa}{N}\right) < 2\cos\gamma \tag{38}$$

which corresponds in the isotropic limit ($\gamma \to 0$) and with (23) to

$$1 > N\cos^2\frac{\pi Q_\kappa}{N} = N\sin^2\frac{\pi(\kappa + \frac{1}{2})}{N} \tag{39}$$

given by Eßler *et al* (1991, 1992). By virtue of $S = N/2 - 2$, the relation (38) can be rewritten as

$$\gamma_{\rm crit} = f(S) = \arccos\left(\frac{S+2}{S+1}\sin\pi\frac{S+1-2\kappa}{2S+4}\right). \tag{40}$$

According to (40), we find for any $S \geqslant 2$ a critical anisotropy with $\gamma < \pi/2$ and, vice versa; for any fixed γ we obtain 'degenerate' solutions described by a spin $S > S_{\rm crit}^{\rm min}$. Although this is exact only for $r = 2$ (and for arbitrary N), there is a good agreement with the numerical results for $r > 2$ and small lattice length ($N < 100$). Thus according to (40), the general behaviour of the lower critical limit should be $S_{\rm crit}^{\rm min} \sim f^{-1}(\gamma)$. In the isotropic limit ($\pi/\gamma = p \to \infty$) and for fixed N, the upper critical boundary (32) tends to infinity and the lower one to a finite value, as is found for the XXX chain in the previous sections.

Due to the estimate (35), the quantity $S_{\rm crit}^{\rm max}$ is independent of N in opposition to $S_{\rm crit}^{\rm min}$. But the critical sectors do not vanish in the thermodynamical limit $N \to \infty$ (that means $S_{\rm crit}^{\rm max} - S_{\rm crit}^{\rm min} > 0$) since we can always find a certain γ which ensures the estimate (35) with $\nu_{\kappa_1} - \nu_{\kappa_2} \gg 1$. In figure 8 the maximum of $p_{\rm crit} = f(S, N)$ is shown for $S = 8$, $\kappa = 1$ as a function of N having a finite asymptotic value $p_{\rm crit}(N \to \infty) = 17.0 \pm 0.5$, which is indeed larger than the minimal value $p_{\rm crit}^{min} = (S+1)/\kappa = 9$ determined by (32). Similar relations should hold for all $S \geqslant 2$. In the thermodynamical limit we can assume therefore non-vanishing critical sectors. For any finite p critical sectors are found with *finite spins*, i.e. 'degenerate' states with a zero magnetization. In the XXX case (where p tends to infinity), this remains unclear. After taking the limit $N \to \infty$, the relation $S_{\rm crit}^{\rm max} - S_{\rm crit}^{\rm min} > 0$ does not imply that $S_{\rm crit}^{\rm min}$ is finite because $S_{\rm crit}^{\rm max}$ tends to infinity too for $p \to \infty$. However, we can choose a number $1 \ll \pi/\gamma = p < \infty$ which is arbitrarily close to the infinite isotropic chain so as to obtain 'degenerate' states with a finite spin.

5. Finite-size corrections

The finite-size corrections to the eigenvalues of a transfer matrix were shown (Cardy 1987, Domb and Green 1976) to depend on the scaling indices and the conformal anomaly of a system with second-order phase transitions (a so-called critical system). A check of the validity of (9)–(11), which are based on the conformal invariance, consists in a calculation of excitations for a solvable model determined by BAE. Several methods were used to obtain analytic corrections. Nevertheless, the first uniform consideration for calculating all lowest-lying excitations of a critical system was developed by Woynarovich and Eckle (1987), who applied the Euler–MacLaurin formula and the Wiener–Hopf integration in the BAE of the anisotropic XXZ model. The authors replace the sum in the BAE (7) by the Euler–MacLaurin formula

$$\int_a^{a+nh} f(x)\,\mathrm{d}x = h\sum_{k=0}^{n} f(a+kh) + R \tag{41}$$

$$R = -\frac{h}{2}\left(f(a+nh) + f(a)\right) - B_2\frac{h^2}{2!}\left(f'(a+nh) - f'(a)\right) - B_4\frac{h^4}{4!}\left(f^{(3)}(a+nh) - f^{(3)}\right) - \ldots \tag{42}$$

where B_k are the Bernoulli numbers. We treat the spin chain (including the 'degenerate' solutions) without any magnetic field. The presence of an external magnetic field leads to complications in the analytical estimations since general values of a non-zero magnetization are connected with non-conformal finite-size effects (Woynarovich *et al* 1989). Though the behaviour of 'degenerate' solutions is clear for the infinite anisotropic chain only, the isotropic case will be investigated at first because it is easier to treat than the XXZ chain: however, the principal way does not differ from the XXZ case.

It is useful to consider the derivative of $z(\lambda)$

$$\sigma_N(\lambda) = A_{1/2}(\lambda) - \frac{1}{N}\sum_{k=1}^{r} A_1(\lambda - \lambda_k) \tag{43}$$

$$A_\kappa(\lambda) = \frac{\kappa}{\pi\left(\lambda^2 + \kappa^2\right)} \tag{44}$$

representing the root density. By substituting $h = 1/N$, $x = z$ and

$$a + kh = \frac{Q_k}{N} \tag{45}$$

the equations (41) and (42) are rewritten as

$$\int_{\Lambda^-}^{\Lambda^+} \sigma_N(\lambda) f(\lambda)\, d\lambda = \frac{1}{N}\sum_{k=1}^{r} f(\lambda_k) + R \tag{46}$$

$$\lambda_k = z^{-1}\left(\frac{Q_k}{N}\right) \tag{47}$$

$$R = -\frac{1}{2N}\left(f(\Lambda^+) + f(\Lambda^-)\right) - \frac{1}{12N^2}\left(\frac{f'(\Lambda^+)}{\sigma_N(\Lambda^+)} - \frac{f'(\Lambda^-)}{\sigma_N(\Lambda^-)}\right) - \dots \tag{48}$$

We point out therefore that due to (47) the z-function (12) has to be monotone. All solutions (roots as well as holes) must lie within the interval $[Q_{\Lambda^-}, Q_{\Lambda^+}]$ with $Q_{\Lambda^\pm} \leftrightarrow \Lambda^\pm$. Hence, there are two possibilities to convert the sum over roots (7) to an integral. Either one splits up the holes

$$\int_{\Lambda_{\min}}^{\Lambda_{\max}} \sigma_N(\lambda) f(\lambda)\, d\lambda = \frac{1}{N}\sum_{k=1}^{r} f(\lambda_k) + \frac{1}{N}\sum_{k=1}^{h} f(\lambda_{\text{hole}}) + R \tag{49}$$

considering the full interval $[Q_{\min}, Q_{\max}]$, or one takes into account only roots within $[Q_{\Lambda^-}, Q_{\Lambda^+}] \subset [Q_{\min}, Q_{\max}]$, where holes are not permitted. That means that the holes lie on the edge of the set $\{Q_k\}$, and the remaining roots out of $[Q_{\Lambda^-}, Q_{\Lambda^+}]$ must be computed by an additional term. The first version was used by Woynarovich (1987b). Many difficulties appear, however, if the function $z(\lambda)$ begins to oscillate and virtual holes occur. We prefer the second point of view, where $z(\lambda)$ may be monotone, provided that the choosen interval $[Q_{\Lambda^-}, Q_{\Lambda^+}]$ does not possess repeating integers. Outside it, a non-monotone behaviour is allowed with some repeating or non-repeating quantum numbers for roots. Holes are of no interest. Hence, we obtain from (7) and (46)

$$\sigma_N(\lambda) + \int_{\Lambda^-}^{\Lambda^+} \sigma_N(\lambda') A_1(\lambda - \lambda')\, d\lambda' = A_{1/2}(\lambda) - \frac{1}{N}\sum_{k=1}^{r^\pm} A_1(\lambda - \lambda_r^\pm) + R. \tag{50}$$

The number $r^\pm$ denotes the roots out of $[Q_{\Lambda^-}, Q_{\Lambda^+}]$. As a normalization condition, the equation

$$\frac{Q_\infty - Q_{\lambda_k}}{N} = \int_{\lambda_k}^{\infty} \sigma_N(\lambda)\, d\lambda \tag{51}$$

is given. If we assume that for large N the roots $\Lambda^\pm$ behave like $\pm \ln N$, we can write $(\lambda \geqslant \Lambda^+ \gg \Lambda^-)$

$$\sigma_N(\lambda) + \int_{-\infty}^{\Lambda^+} \sigma_N(\lambda') A_1(\lambda - \lambda')\, d\lambda' \cong A_{1/2}(\lambda) - \frac{1}{N}\sum_{k=1}^{r^+} A_1(\lambda - \lambda_r^+) + R \tag{52}$$

which is a special form of a Wiener–Hopf integral equation (Fenyo and Stolle 1983):

$$\chi(s) - \int_0^{+\infty} P(s - t)\chi(t)\, dt = f(s). \tag{53}$$

This equation was solved by some authors (Woynarovich and Eckle 1987, Hamer *et al* 1987). One can factorize the Fourier-transformed kernel into two continuous functions $\hat{g}_{\pm}(\omega)$ which are holomorphic in the lower and upper halves of the complex plane, respectively.

$$1-\hat{P}(\omega)=\frac{1}{\hat{g}_{+}(\omega)\hat{g}_{-}(\omega)}. \tag{54}$$

Then the general solution in the ω-space reads

$$\hat{\chi}_{+}(\omega)=\hat{g}_{+}(\omega)\int\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}\frac{\hat{g}_{-}(\omega')\hat{f}(\omega')}{\omega-\omega'-\mathrm{i}0}. \tag{55}$$

For a proof see e.g. Karowski (1988). The factorizations for the isotropic Heisenberg model are fairly complicated

$$\hat{g}_{\pm}(\omega)=\exp\left(\pm\int\frac{\mathrm{d}\omega'}{2\pi\mathrm{i}}\frac{\ln(1+\mathrm{e}^{-|\omega'|})}{\omega-\omega'\mp\mathrm{i}0}\right) \tag{56}$$

$$=\frac{\sqrt{2\pi}}{\Gamma\left(1/2\mp\omega/2\pi\mathrm{i}\right)}\exp\left[\mp\frac{\omega}{2\pi\mathrm{i}}\left(\ln\left(0\mp\omega/2\pi\mathrm{i}\right)-1\right)\right] \tag{57}$$

and it seems to be almost impossible to calculate analytically a solution for $\sigma_N(\lambda)$. There are two points: the correction R in (41) is treatable up to the second order in h. Fortunately that restriction is sufficient for computing the first order of finite-size corrections (Karowski 1988). Furthermore, the rapidities of roots or holes respectively which are treated separately are unknown and they are only implicitly determined by (51). Yet Woynarovich and Eckle succeeded in describing the lowest excitations by also replacing the sum in the energy formula (4) by the Euler–MacLaurin equation in the same way. All unknown and untreatable terms cancel. We deal with the BAE of the XXX model with exactly the same methods introduced for the XXZ spin chain in the paper of Woynarovich (1987a, 1987b), although with one exception that is described above in order to include repeating quantum numbers. For real magnons we obtain (cf Jüttner 1992) a formula for the gap between the finite and the infinite system which holds both for the XXX and XXZ chain.

$$E_N-E_\infty=\frac{\pi^2}{2N}\left[\left(\frac{Q_\infty-Q_{\Lambda^+}-1/2}{\hat{g}(0)}\right)^2+\left(\frac{Q_{\Lambda^-}-Q_{-\infty}-1/2}{\hat{g}(0)}\right)^2\right]$$
$$+\frac{\pi^2}{N}\left(-\frac{1}{12}+M^{+}+M^{-}\right) \tag{58}$$

$$M^{\pm}=\pm\sum_{k=1}^{r^{\pm}}(Q_k^{\pm}-Q_{\Lambda^{\pm}})-\frac{r^{\pm}(r^{\pm}+1)}{2}. \tag{59}$$

Equation (57) gives one the constant $\hat{g}(0)$ which is the limit $\gamma\to 0$ of the general factorization for the XXZ model (cf Hamer *et al* 1987)

$$\hat{g}(0)=\sqrt{2(1-\gamma/\pi)}. \tag{60}$$

Defining now an integral number Δ playing the role of the asymmetry with respect to the set $\{Q_k\}$,

$$\Delta=\frac{Q_\infty-Q_{\Lambda^+}-r^+}{2}-\frac{Q_{\Lambda^-}-Q_{-\infty}-r^-}{2} \tag{61}$$

the finite-size corrections read

$$E_N - E_\infty = -\frac{\pi^2}{12N} + \frac{\pi^2}{N}\left(\frac{1-\gamma/\pi}{2}S^2 + \frac{1}{2(1-\gamma/\pi)}\Delta^2 + M^+ + M^-\right) \tag{62}$$

$$P_N - P_\infty = -\pi(S+\Delta) + \frac{2\pi}{N}(-S\Delta - M^+ + M^-). \tag{63}$$

Note that the dispersion relation (62), (63) (which corresponds to $c = 1$) is also valid for repeating quantum numbers Q_k. The excitations (62) can be easily fitted into the conformal scheme (9), (10) with scaling indices of Gaussian form:

$$x = \frac{1-\gamma/\pi}{2}S^2 + \frac{1}{2(1-\gamma/\pi)}\Delta^2 \qquad l = -S\Delta. \tag{64}$$

In the non-degenerate case a redefinition of S, Δ and $M^\pm$ is possible and one obtains the same numbers used in the preprint of Woynarovich (1987b). We also took into consideration complex roots. There is another determination of S, Δ and $M^\pm$ because of the necessary distinction of complex roots in to so-called close and wide pairs ($|\,\mathrm{Im}\lambda_k\,| < 1$ or $|\,\mathrm{Im}\lambda_k\,| > 1$, respectively). Woynarovich included a real root with an integer greater than Q_∞ by an additional calculation of a complex root with an imaginary part tending to zero. But in the limit, the function $z(\lambda)$ oscillates. It was therefore useful to investigate real roots separately. However, in principle neither the dispersion relation nor the complex roots are changed by the new type of real solutions.

6. Conclusions

Real solutions with identical quantum numbers in the logarithmic form of the Bethe ansatz equations for the spin-$\frac{1}{2}$ Heisenberg chain appear in excitated states, as compared with the antiferromagnetic ground state which can be characterized by the total spin S of the chain. The spin of configurations with double roots (i.e. two roots have the same integer) was found to lie in critical sectors that are functions of the anisotropy γ and the position of the quantum number of the double root described by κ. The remaining roots as well as the lattice length depend on it only slightly. Furthermore, in the thermodynamical limit (infinite lattice length), the critical spin may be finite, which implies zero magnetization. However, the structure of the finite-size corrections is not influenced by the appearance of such solutions.

Since we do not take complex roots into consideration (with respect to the existence of 'degenerate' solutions), we are not able to give an answer about a possible disappearance of complex solutions and about their relation to the new real roots. Thus the total number of all real and complex configurations determined by N and r is unclear. It is generally believed, however, that the Bethe ansatz solutions for the XXX model are complete.

Though the real rapidities with identical integers are not distinguishable from a 'normal' real root with respect to the algebraic BAE—where the integers do not occur—they are said to be 'degenerate' solutions with respect to the logarithmic BAE. The number of holes is shown to depend on the set $\{Q_k\}$ and it is not fixed by the spin. Therefore, the usual classification of the spin by the number of holes meets difficulties.

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