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Degenerated ground states and excited states of the $S = \frac{1}{2}$ anisotropic antiferromagnetic Heisenberg chain in the easy axis region

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Abstract. We reconsider the solutions of the Bethe ansatz equations for the antiferromagnetic XXZ model in the easy axis region. The excitations are obtained by leaving holes in the ground state distribution of the momenta and allowing for complex rapidities. Equations for the parameters of the holes are given and it is shown that the higher level equations contrary to earlier results have the same structure as in the planar region. The existence of degenerate ground states is demonstrated, and it is also shown, that distinct sets of excited states with analogous structure exist above both ground states.

1. Introduction

For almost twenty years attempts have been made to offer a better means of understanding the excited states of the anisotropic Heisenberg model in the antiferromagnetic case.

The Hamiltonian of the problem is:

$$H = \sum_{n=1}^N \{S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \rho S_n^z S_{n+1}^z\} \quad (1)$$

with periodic boundary conditions, N is assumed to be even, S_n^x , S_n^y , S_n^z are the components of spin- $\frac{1}{2}$ operators.

In order to describe the eigenstates of (1) the Bethe ansatz is generally used (Bethe 1931). The ground state is known to be described by real momenta $\{k_j\}$ and the corresponding equidistant set of integers (or half-odd integers) appearing in Bethe ansatz equations (Yang and Yang 1966). The excited states are sought by leaving holes in the integer (or half-odd integer) set and by allowing complex wavenumbers.

Des Cloizeaux and Gaudin (1966) investigated the spin-wave states of the system and Johnson *et al* (1973) found the dispersion relation for the low-lying excitations using the results for the transfer matrix of the eight-vertex model.

Recently Woynarovich (1982) in part of the planar region, and Babelon *et al* (1983a hereafter referred to as bvv) in the whole antiferromagnetic region analysed the Bethe ansatz equations of the XXZ model. They expressed the density of real roots by the

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parameters of holes and complex rapidities and found a system of coupled equations containing only the parameters of the excitations.

It is well known (Orbach 1958, Babelon *et al* 1983b) that in the region $\rho > 1$ the antiferromagnetic ground state is two-fold degenerate when $N \rightarrow \infty$. Orbach has pointed out that these two ground states correspond to two sets of integers both increasing by two and shifted by one relative to each other (see equation (3) of the present paper). If one calculates only the density of the real roots then no distinction can be made between these two states.

Our aim is to investigate how this 'second' ground state and also the excitations above it can be obtained from Bethe ansatz equations and what is the difference between the two types of excitations.

Our method is similar to that used by Woynarovich (1982) and we express the values of the real rapidities themselves because this enables us to distinguish between the two types of states. The main point is that we fix the boundaries of the region containing the real roots—but only at the end of the calculation thus avoiding the loss of certain solutions.

In this way we obtain the two degenerated ground states and the excitations above them. We write down the equations for the parameters of the holes as well and it turns out that the allowed values of these parameters are different for the two types of excitations. The difference is of the order of $1/N$. The structure of these excitations and their spectrum are the same as found by *bv*v, so the two types of excitations become degenerate in the $N \rightarrow \infty$ limit like the ground states.

During the calculations it turns out that the higher level equations for the complex roots take a simpler form than found by *bv*v and so the structure of these equations is the same for the whole antiferromagnetic region $-1 < \rho < \infty$.

In § 2 we introduce the general formalism; in § 3 we rederive the density of real rapidities but do not fix the boundaries of the region (only its length) that will contain the real roots. This allows us to obtain the ground state and excitations of the second type. Section 4 gives the higher level equations in simpler form, and the equations for the holes and the real roots; the differences between the two types of states are discussed. In § 5 we deal with the energy and momentum of these states, and we provide a summary of our results in § 6.

2. Formalism

It is well known that (1) can be diagonalised by Bethe's ansatz (see for e.g. Orbach 1958) if the phases and momenta satisfy the following set of coupled equations:

$$\cot \frac{1}{2}\psi_{\alpha\beta} = -\rho \frac{\cot \frac{1}{2}k_{\alpha} - \cot \frac{1}{2}k_{\beta}}{(1-\rho) \cot \frac{1}{2}k_{\alpha} \cot \frac{1}{2}k_{\beta} - (1+\rho)} \quad (2)$$

$$Nk_{\alpha} = 2\pi\lambda_{\alpha} + \sum_{\beta \neq \alpha} \psi_{\alpha\beta}, \quad \lambda_{\alpha} \text{ integer} \quad (3)$$

where $\alpha, \beta = 1, \dots, r$ and r is connected with the total spin projection $S^z = \frac{1}{2}N - r$. Moreover the following conventions are used:

$$0 \leq \text{Re } k < 2\pi, \quad -\pi < \text{Re } \psi \leq \pi. \quad (4)$$

The energy and momentum of a state are given by

$$E - E_F = \sum_{\alpha=1}^r (\cos k_\alpha - \rho), \quad K = \sum_{\alpha=1}^r k_\alpha. \tag{5}$$

Here $E_F = \frac{1}{4}N\rho$ is the energy of the ferromagnetic state.

In order to solve the system of equations (2), (3) it is useful to introduce auxiliary variables, the so-called rapidities. In the case $\rho > 1$ the following choice is suitable (Walker 1959):

$$\rho = \cosh \gamma, \quad 0 < \gamma < \infty \tag{6}$$

$$\cot \frac{1}{2}k_\alpha = \coth \frac{1}{2}\gamma \tan \eta_\alpha. \tag{7}$$

Here $\text{Re } \eta$ for the sake of unicity is restricted to an interval of length π , but the ends of this interval are not fixed at this stage.

Moreover let us define the following function:

$$\phi(z, \alpha) = -i \ln \frac{\sin(z + i\alpha)}{\sin(z - i\alpha)} = 2 \cot^{-1}(\coth \alpha \tan z) \tag{8}$$

where the cut of the \ln function is on the positive real semiaxis. Using these variables and functions we can write the Bethe ansatz equations (equations (2), (3)) in a more tractable form:

$$N\phi(\eta_\alpha, \frac{1}{2}\gamma) = 2\pi I_\alpha + \sum_{\beta=1}^r \phi(\eta_\alpha - \eta_\beta, \gamma) \tag{9}$$

where I_α is a half-odd integer.

The energy and momentum can be expressed by the rapidities

$$E - E_F = \frac{\sinh \gamma}{2} \sum_{\alpha=1}^r \phi'(\eta_\alpha, \frac{1}{2}\gamma), \quad K = \sum_{\alpha=1}^r \phi(\eta_\alpha, \frac{1}{2}\gamma) \tag{10}$$

where $\phi'(z, \alpha) = (\partial/\partial z)\phi(z, \alpha)$.

We shall use the Fourier expansion of the above functions

$$\phi'(z, \alpha) = \sum_{m=-\infty}^{\infty} \tilde{\phi}'_m(y, \alpha) e^{2imx}, \quad z = x + iy \tag{11}$$

where

$$\tilde{\phi}'_m(y, \alpha) = \begin{cases} y > \alpha: & 4 \sinh(2\alpha|m|) e^{-2ym} & \text{if } m > 0, 0 \text{ otherwise} \\ |y| < \alpha: & -2 e^{-2\alpha|m|} e^{-2ym} \\ y < -\alpha: & 4 \sinh(2\alpha|m|) e^{-2ym} & \text{if } m < 0, 0 \text{ otherwise} \end{cases} \tag{12}$$

and

$$\phi(z, \alpha) = \sum_{m \neq 0} \frac{\tilde{\phi}'_m(y, \alpha)}{2im} e^{2imx} + \begin{cases} y > \alpha: & -2i\alpha + 2\pi f_1(x) \\ |y| < \alpha: & \pi - 2z + 2\pi f_2(x) \\ y < -\alpha: & 2i\alpha + 2\pi f_1(x). \end{cases} \tag{13}$$

Here $f_1(x)$ and $f_2(x)$ are functions taking only integer values:

$$\left. \begin{aligned} f_1(x) &= \begin{cases} 1 & \text{if } (2n-1)\pi/2 < x < 2n\pi/2 \\ 0 & \text{if } 2n\pi/2 < x < (2n+1)\pi/2 \end{cases} \\ f_2(x) &= n & \text{if } (2n-1)\pi/2 < x < (2n+1)\pi/2 \end{aligned} \right\} n \text{ integer.} \tag{14}$$

3. The equations for the real rapidities

In this section we rederive the expression for the density of real roots and give a formula for the rapidities themselves. It is known that the complex roots appear in conjugated pairs ($\eta_i = \sigma_i \pm i\tau_i, \tau_i > 0$) and it is necessary to make a distinction between close ($\tau_c < \gamma$) and wide ($\tau_w > \gamma$) pairs (BVV).

If M, N_c, N_w represent the number of real roots, close and wide pairs, respectively, equations (9) for the real roots take the form:

$$\begin{aligned}
 N\phi(\eta_j, \frac{1}{2}\gamma) &= 2\pi I_j + \sum_{i=1}^M \phi(\eta_j - \eta_i, \gamma) \\
 &+ \sum_{c=1}^{N_c} [\phi(\eta_j - \eta_{c_s}, \gamma) + \phi(\eta_j - \bar{\eta}_{c_s}, \gamma)] \\
 &+ \sum_{w=1}^{N_w} [\phi(\eta_j - \eta_{w_s}, \gamma) + \phi(\eta_j - \bar{\eta}_{w_s}, \gamma)].
 \end{aligned}
 \tag{15}$$

Using the Fourier expansion (13) we get:

$$\sum_{m \neq 0} \frac{e^{2im\eta_j}}{2im} A_m + \frac{N - M - 2N_c}{N} (\pi - 2\eta_j) - \frac{2}{N} \left(\sum_{i=1}^M \eta_i + 2 \sum_{c=1}^{N_c} \sigma_c \right) = 2\pi \frac{I'_j}{N}
 \tag{16}$$

where

$$\begin{aligned}
 A_m &= \tilde{\phi}'_m(0, \frac{1}{2}\gamma) - \frac{1}{N} \left(\tilde{\phi}'_m(0, \gamma) \sum_{i=1}^M e^{-2im\eta_i} \right. \\
 &+ \sum_{c=1}^{N_c} e^{-2im\sigma_c} [\tilde{\phi}'_m(-\tau_{c_s}, \gamma) + \tilde{\phi}'_m(\tau_{c_s}, \gamma)] \\
 &\left. + \sum_{w=1}^{N_w} e^{-2im\sigma_w} [\tilde{\phi}'_m(-\tau_{w_s}, \gamma) + \tilde{\phi}'_m(\tau_{w_s}, \gamma)] \right)
 \end{aligned}
 \tag{17}$$

and

$$I'_j = I_j - Nf_2(\eta_j) + \sum_{i=1}^M f_2(\eta_j - \eta_i) + 2 \sum_{c=1}^{N_c} f_2(\eta_j - \sigma_c) + 2 \sum_{w=1}^{N_w} f_1(\eta_j - \sigma_w)
 \tag{18}$$

is again a half-odd integer.

The left-hand side of (16) is the sum of a linear and a periodic function and is a monotonically decreasing (if N is large) continuous function of η_j . All the real roots must fall within an interval of length π . This requirement restricts the number P of the half-odd integers on the right-hand side of (16) which is apparently the sum of the number of real roots and the number of holes N_h in the distribution of real roots:

$$P = N - M - 2N_c = M + N_h
 \tag{19}$$

N is even so N_h is even as well and from (19)

$$M = \frac{1}{2}N - \frac{1}{2}N_h - N_c, \quad P = \frac{1}{2}N + \frac{1}{2}N_h - N_c.
 \tag{20}$$

This determines the spin projection:

$$S^z = \frac{1}{2}N - r = \frac{1}{2}N - M - 2N_c - 2N_w = \frac{1}{2}N_h - N_c - 2N_w.
 \tag{21}$$

Note that the beginning (or end) of the I' half-odd integer set is not fixed yet.

We can now suppose that $\eta(x): \mathbb{R} \rightarrow \mathbb{R}$ is a continuous monotonically decreasing function for which

$$\eta_j = \eta(I'_j / N) \tag{22}$$

Then the RHS of (16) takes the form $2\pi\eta^{-1}(\eta_j)$. Let us require that (16) holds not only for the real roots η_j but for all real values w . This gives us the possibility to determine the unknown $\eta^{-1}(w)$ function

$$\sum_{m \neq 0} \frac{e^{2imw}}{2im} A_m + \frac{P}{N}(\pi - 2w) - \frac{2}{N} \left(\sum_{i=1}^M \eta_i + 2 \sum_{c=1}^{N_c} \sigma_c \right) = 2\pi\eta^{-1}(w). \tag{23}$$

Taking the derivative of (23) with respect to w we get

$$\sum_{m=-\infty}^{\infty} A_m e^{2imw} = 2\pi\sigma(w) \tag{24}$$

where $\sigma(w) = (d/dw)\eta^{-1}(w)$ is apparently a periodic function

$$\sigma(w) = \sum_{m=-\infty}^{\infty} \tilde{\sigma}_m e^{2imw}. \tag{25}$$

Then, from (24), we see that

$$A_m = 2\pi\tilde{\sigma}_m. \tag{26}$$

Remember that A_m contains $\tilde{\sigma}_m$ through the sum over real roots (see (17)):

$$\begin{aligned} \sum_{i=1}^M e^{-2im\eta_i} &= \sum_{i=1}^M \exp\left\{-2im\eta\left(\frac{I'_i}{N}\right)\right\} \\ &= \sum_{j=1}^P \exp\left\{-2im\eta\left(\frac{I'_j}{N}\right)\right\} - \sum_{h=1}^{N_h} e^{-2im\Theta_h} \end{aligned} \tag{27}$$

where

$$\Theta_h = \eta(I'_{j_h} / N) \tag{28}$$

is the parameter of a hole in the I' set ($h = 1, \dots, N_h$), and $I'_j = I'_p + P - j$. The first term of the RHS of (27) can be rewritten in integral form using the formula

$$\frac{1}{N} \sum_{I=I_{\min}}^{I_{\max}} f\left(\frac{I}{N}\right) = \int_{(I_{\min}-\frac{1}{2})/N}^{(I_{\max}+\frac{1}{2})/N} dx f(x) + O\left(\frac{1}{N^2}\right). \tag{29}$$

After changing the variable of integration we get:

$$\begin{aligned} \sum_{i=1}^M e^{-2im\eta_i} &= - \sum_{h=1}^{N_h} e^{-2im\Theta_h} - N \int_{\eta_{\min}}^{\eta_{\max}} dy \sigma(y) e^{-2imy} \\ &= - \sum_{h=1}^{N_h} e^{-2im\Theta_h} - N\pi\tilde{\sigma}_m \end{aligned} \tag{30}$$

where

$$\eta_{\min} = \eta(I'_1 / N + 1/2N), \quad \eta_{\max} = \eta(I'_p / N - 1/2N) \tag{31}$$

are the boundaries of the interval containing the real roots and it is assumed that $\eta_{\max} - \eta_{\min} = \pi$.

Now $\tilde{\sigma}_m$ can be evaluated from (26)

$$\tilde{\sigma}_m = -\frac{1}{2\pi} \frac{1}{\cosh(\gamma m)} \left[1 - \frac{1}{N} e^{-\gamma|m|} \left(\sum_{c=1}^{N_c} e^{-2im\sigma_c} (e^{2m\tau_c} + e^{-2m\tau_c}) \right) - (e^{4\gamma|m|} - 1) \sum_{w=1}^{N_w} e^{-2im\sigma_w} e^{-2\tau_w|m|} - \sum_{h=1}^{N_h} e^{-2im\Theta_h} \right]. \tag{32}$$

This expression is proportional to the regular density of real roots derived by *bvv* (the coefficient is $-N$). $\tilde{\sigma}_m$ contains only the complex roots and the holes as parameters. We are now able to determine the $\eta^{-1}(w)$ function on the RHS of (23) after evaluating the sum of real roots on the LHS of (23) in the same manner as in (30)

$$\sum_{i=1}^M \eta_i = -\sum_{h=1}^{N_h} \Theta_h - N\pi \left(\sum_{m \neq 0} \frac{e^{2im\eta_{\max}}}{2im} \tilde{\sigma}_m + \frac{P}{2\pi N} (\pi - 2\eta_{\max}) \right) \tag{33}$$

Then

$$\eta^{-1}(w) = \sum_{m \neq 0} \frac{\tilde{\sigma}_m}{2im} (e^{2imw} + e^{2im\eta_{\max}}) + \frac{P}{2\pi N} [2\pi - 2(w + \eta_{\max})] + \frac{1}{\pi N} \left(\sum_{h=1}^{N_h} \Theta_h - 2 \sum_{c=1}^{N_c} \sigma_c \right). \tag{34}$$

Equations (31) must be satisfied, so

$$\sum_{m \neq 0} \frac{e^{2im\eta_{\max}}}{2im} \tilde{\sigma}_m + \frac{P}{2\pi N} (\pi - 2\eta_{\max}) = \frac{I'_p - \frac{1}{2}}{2N} - \frac{1}{2\pi N} \left(\sum_{h=1}^{N_h} \Theta_h - 2 \sum_{c=1}^{N_c} \sigma_c \right). \tag{35}$$

This equation determines η_{\max} if I'_p (the smallest element of the I' set) is given. Using (35), (34) can be written in the form

$$\eta^{-1}(w) = \sum_{m \neq 0} \frac{e^{2imw}}{2im} \tilde{\sigma}_m + \frac{P}{2\pi N} (\pi - 2w) + \frac{1}{2\pi N} \left(\sum_{h=1}^{N_h} \Theta_h - 2 \sum_{c=1}^{N_c} \sigma_c \right) + \frac{I'_p - \frac{1}{2}}{2N}. \tag{36}$$

This expression will be further simplified and used in § 4.

4. Higher level equations, equations for the holes and for the real roots

Equations (9) for the complex roots can be written in exponential form:

$$\exp i \left(N\phi(\eta_b, \frac{1}{2}\gamma) - \sum_{i=1}^M \phi(\eta_i - \eta_b, \gamma) - \sum_{c=1}^{N_c} [\phi(\eta_i - \eta_{c_s}, \gamma) + \phi(\eta_i - \bar{\eta}_{c_s}, \gamma)] - \sum_{w=1}^{N_w} [\phi(\eta_i - \eta_{w_s}, \gamma) + \phi(\eta_i - \bar{\eta}_{w_s}, \gamma)] \right) = -1. \tag{37}$$

The sum containing the real roots can be evaluated straightforwardly using the Fourier expansion (13) and the density of the real roots (32).

If η_i is a wide root we obtain:

$$\exp\{iG(\eta_w)\} = -1 \tag{38}$$

where

$$\begin{aligned}
 G(z) = & - \sum_{h=1}^{N_h} \phi(z - \Theta_h - i\frac{1}{2}\gamma, \frac{1}{2}\gamma) \\
 & + \sum_{c=1}^{N_c} [\phi(z - \eta_c - i\frac{1}{2}\gamma, \frac{1}{2}\gamma) + \phi(z - \bar{\eta}_c - i\frac{1}{2}\gamma, \frac{1}{2}\gamma)] \\
 & + \sum_{w=1}^{N_w} [\phi(z - \eta_w, \gamma) + \phi(z - \bar{\eta}_w - i\gamma, \gamma)].
 \end{aligned}
 \tag{39}$$

This is the result of *bvv*.

Since the density of the real roots is the same as found by *bvv*, the evaluation of the sum over the real roots in (37) leads—in the same way as in *bvv*—to the conclusion that the close roots must have quartet or two-string structure. Utilising this property of the close roots and then equation (35) we find also for the close roots

$$\exp\{iG(\eta_c)\} = -1.
 \tag{40}$$

It is remarkable that the δ term in equation (23) of *bvv* vanishes as a consequence of (35).

Let us introduce the set of parameters $\{\chi_j\}_{j=1}^{\mathcal{P}}$ for the complex roots as in *bvv*, namely

$$\chi = \begin{cases} z - i\frac{1}{2}\gamma & \text{for a two-string } (z, \bar{z} = z - i\gamma) \\ \sigma \pm i(\tau - \frac{1}{2}\gamma) & \text{for a quartet } (z = \sigma + i\tau, \bar{z}, z - i\gamma, \bar{z} + i\gamma, \frac{1}{2}\gamma < \tau < \gamma) \\ \sigma \pm i(\tau - \frac{1}{2}\gamma) & \text{for a wide pair } (\sigma + i\tau, \sigma - i\tau, \tau > \gamma). \end{cases}
 \tag{41}$$

The number of these parameters is

$$\mathcal{P} = N_{\text{string}} + 2N_{\text{quartet}} + 2N_w = N_c + 2N_w.
 \tag{42}$$

We can see from (21) and (42) that

$$S^z = \frac{1}{2}N_h - \mathcal{P}.
 \tag{43}$$

If the $\{\chi_j\}$ set is used, the equations for the complex roots ((38) and (40)) read

$$\prod_{h=1}^{N_h} \frac{\sin(\chi_j - \Theta_h + i\frac{1}{2}\gamma)}{\sin(\chi_j - \Theta_h - i\frac{1}{2}\gamma)} = - \prod_{i=1}^{\mathcal{P}} \frac{\sin(\chi_j - \chi_i + i\gamma)}{\sin(\chi_j - \chi_i - i\gamma)}.
 \tag{44}$$

Thus the higher level equations have a structure analogous to that in the planar case, i.e. in a wider sense they have the same structure for the whole antiferromagnetic region.

Let us now return to the evaluation of the *rhs* of (36). This can be carried out in a straightforward manner with the help of (32) and utilising the quartet (or two-string) structure of the close roots:

$$\begin{aligned}
 \eta^{-1}(w) = & \frac{I'_P - \frac{1}{2}}{2N} + \frac{1}{4} - \frac{1}{2\pi} \operatorname{am}\left(\frac{2K}{\pi}w, k\right) \\
 & - \frac{1}{2\pi N} \left(\sum_{j=1}^{\mathcal{P}} [\phi(w - \chi_j, \frac{1}{2}\gamma) - 2\pi f_i(w - \operatorname{Re} \chi_j)] \right) \\
 & + \sum_{h=1}^{N_h} [\mathcal{F}(w - \Theta_h, \gamma) - \frac{1}{2}\pi]
 \end{aligned}
 \tag{45}$$

Here $\operatorname{am}(u, k)$ is the Jacobian elliptic function; K is the complete elliptic function of

the first kind with the modulus k for which

$$K'/K = \gamma/\pi \tag{46}$$

and $i = 1$ if χ_j is the parameter of a member of a wide pair and $i = 2$ otherwise. The appearance of functions f_1 and f_2 removes the jumps of the ϕ functions in (45). Moreover:

$$\mathcal{F}(x, \gamma) = x + \sum_{m=1}^{\infty} \frac{e^{-\gamma m}}{m \cosh(\gamma m)} \sin(2mx). \tag{47}$$

Now the equations for the real roots (22) and for the holes (28) read:

$$I'_j/N = \eta^{-1}(\eta_j) \tag{48}$$

$$I'_{j_h}/N = \eta^{-1}(\Theta_h). \tag{49}$$

Equations (44) and (49) are a closed system of equations for the variables χ_j and Θ_h . Once this system is solved through (41) the complex roots, and by (48) the real roots can be found.

In discussing the possible solutions attention must be paid to the fact, that in equation (49) (and also in (48)) in addition to the parameters of the holes I'_{j_h} (parameters of the real roots I'_j) an extra parameter I'_p appears, moreover it appears in the form $(I'_p - \frac{1}{2})/(2N)$. Due to this, the decreasing or increasing of I'_p , i.e. the lower boundary of the I' set by one has the same effect on the solution as shifting the whole I' set by a half. This indicates that equations (48) and (49) may have different solutions for different values of I'_p . Remember that we have no explicit restriction for the boundaries of the I' set. The only requirement is that the rapidities and the parameters of the holes must fall within an interval of length π . If this interval is given, for example, by

$$-\frac{1}{2}\pi < \eta_j, \quad \Theta_h, \quad \text{Re } \chi_j \leq \frac{1}{2}\pi \tag{50}$$

we can find different solutions for different values of I'_p which satisfy (50).

The simplest example is given by the two ground states which are characterised by $N_h = 0, \mathcal{P} = 0$ so $P = M = \frac{1}{2}N$ and $S^z = 0$. From (48) and (45) we obtain:

$$\eta_j = \eta\left(\frac{I'_j}{N}\right) = \frac{\pi}{2K} F\left[\frac{2\pi}{N}\left(j - \frac{I'_p + \frac{1}{2}}{2}\right) - \frac{1}{2}\pi, k\right], \quad j = 1, \dots, \frac{1}{2}N \tag{51}$$

where $F(\varphi, k)$ is the elliptic integral of the first kind and $I'_j = I'_p + P - j$ was used. It can be seen that for $I'_p + \frac{1}{2} = 0$ and for $I'_p + \frac{1}{2} = 1$ we get different solutions both satisfying (50). For other values of $I'_p + \frac{1}{2}$ the solutions will not satisfy (50) or in other words these solutions give the same momentum set $\{k_j\}$ as one of the solutions with $I'_p + \frac{1}{2} = 0$ and 1 because of the periodicity in equation (7).

The two different sets of momenta $\{k_j\}$ can be obtained from (7) and, e.g. for $\gamma \rightarrow 0$ ($\rho \rightarrow 1$), have the form:

$$\begin{aligned} I'_p + \frac{1}{2} = 0: & \quad k_j = 2 \cot^{-1} \left[\frac{2}{\pi} \ln \tan \left(\frac{\pi}{N} j \right) \right] \\ I'_p + \frac{1}{2} = 1: & \quad k_j = 2 \cot^{-1} \left[\frac{2}{\pi} \ln \tan \left(\frac{\pi}{N} (j - \frac{1}{2}) \right) \right]. \end{aligned} \quad j = 1, \dots, \frac{1}{2}N$$

Let us consider the general case! Since it is not known *a priori*, what values of I'_p are compatible to (50), write (49) in exponential form:

$$\begin{aligned}
 & (-1)^{N/2+I_p+1/2} \\
 &= \exp\left\{iN\text{am}\left(\frac{2K}{\pi}\Theta_h, k\right)\right\} \\
 & \times \prod_{j=1}^{\mathcal{P}} \frac{\sin(\Theta_h - \chi_j + i\frac{1}{2}\gamma)}{\sin(\Theta_h - \chi_j - i\frac{1}{2}\gamma)} \prod_{b=1}^{N_p} \exp\{i[\mathcal{F}(\Theta_h - \Theta_b, \gamma) - \frac{1}{2}\pi]\} \tag{52}
 \end{aligned}$$

which shows that only the parity of $I'_p + \frac{1}{2}$ is important. In order to obtain a solution of the Bethe ansatz equations we have to solve (44) and (52) for the complex roots and for the holes with a given parity of $I'_p + \frac{1}{2}$ and with the constraint (50). Then (48) and (50) determine the real roots, together with the actual value of I'_p .

There is however an other possibility, too. Since only the parity of $I'_p + \frac{1}{2}$ is important, and the wavenumbers are periodic functions of the rapidities, we may drop the constraint (50) for the time and fix $I'_p + \frac{1}{2}$ to be 0 or 1. Naturally we will get different rapidity sets but some of them from the group $I'_p + \frac{1}{2} = 0$ may be identical to others from the group $I'_p + \frac{1}{2} = 1$, in the sense that they determine the same momentum set.

In order to avoid this duplication let us examine how two identical sets can belong to different values of $I'_p + \frac{1}{2}$.

Let us suppose that $\{\chi_j\}_{j=1}^{\mathcal{P}}$ and

$$\eta_1 < \eta_2 < \dots < \eta_P \tag{53}$$

are solutions of (44), (48) and (49) with a given I'_p . (Equation (53) contains the real roots and the parameters of the holes as well.) An equivalent set can be constructed by increasing some of the η 's by π . (The $\{\chi_j\}$ set remains the same because (44) does not change when some of the Θ_h 's are increased by π .) This can be done generally in the following way:

$$\eta_{m+1} < \eta_{m+2} < \dots < \eta_P < \eta_1 + \pi < \eta_2 + \pi < \dots < \eta_m + \pi \tag{54}$$

(the η 's must again fall within an interval of length π). It is easy to check that if we shift m η 's including n holes then (54) is a solution of (44), (48) and (49) with I'_p , for which

$$I'_p = I''_p + 2m - n. \tag{55}$$

In our case $I'_p - I''_p = 1$ and as $m \geq n \geq 0$ we get $m = n = 1$. This means that if η_1 in (53) is a parameter of a hole then (53) is equivalent to one of those sets which can be obtained by solving (44), (48) and (49) with $I'_p = I''_p - 1$. This result allows us to determine the number of really different (non-equivalent) solutions to (44), (48) and (49).

In both cases ($I'_p + \frac{1}{2} = 0$ and $I'_p + \frac{1}{2} = 1$) we have $\binom{P}{N_h}$ possibilities for the sites of holes. We have to exclude those solutions from the group $I'_p + \frac{1}{2} = 1$ for which I'_1 belongs to a hole. The number of these states is apparently $\binom{P-1}{N_h-1}$ so the ratio of 'double' solutions to second type solutions is

$$\frac{\binom{P-1}{N_h-1}}{\binom{P}{N_h}} = N_h/P$$

which is of the order of $1/N$ if $N \rightarrow \infty$ while N_h and \mathcal{P} are finite. We conclude that the 'overlapping' of the first and second type solutions vanishes in the $N \rightarrow \infty$ limit.

Once we have all the non-equivalent solutions for $I'_p + \frac{1}{2} = 0$ and 1, in the way described above (see (53) and (54)) all the rapidity sets may be made to satisfy the constraint (50), and at the same time the corresponding I'_p s can be found too (see (55)). If we have all solutions satisfying (50) it is natural to regard those with $I'_p + \frac{1}{2} = \text{even}$ to be excited states above the ground state with $I'_p + \frac{1}{2} = 0$ and those with $I'_p + \frac{1}{2} = \text{odd}$ excited states above the ground state with $I'_p + \frac{1}{2} = 1$. This picture is supported by the structure of the energy and the momenta of the excited states.

5. Energy and momentum

The energy and momentum of a state can be calculated in a straightforward way using (10)–(13), (32) and (35). The energy has the same form as derived by *bvv* and Johnson *et al* (1973):

$$E - E_F = E_0 + \sum_{h=1}^{N_h} \varepsilon(\Theta_h) \quad (56)$$

$$E_0 = -N \sinh \gamma \left(\sum_{m=1}^{\infty} (1 - \tanh(\gamma m)) + \frac{1}{2} \right) \quad (57)$$

$$\varepsilon(x) = \frac{K}{\pi} \sinh \gamma \operatorname{dn} \left(\frac{2K}{\pi} x, k \right), \quad \operatorname{dn}(u, k) = \frac{\partial}{\partial u} \operatorname{am}(u, k). \quad (58)$$

In the momentum I'_p appears:

$$K = K_0 + \sum_{h=1}^{N_h} p(\Theta_h) \quad (59)$$

$$K_0 = \left(\frac{1}{2} N + I'_p - \frac{1}{2} \right) \pi \quad (60)$$

$$p(x) = \operatorname{am} \left(\frac{2K}{\pi} x, k \right) - \frac{1}{2} \pi. \quad (61)$$

In the energies of the two kinds of states there are no explicit differences but the momenta for the two kinds of states differ also explicitly through K_0 . If we regard the holes as some sort of excitations, each excitation has the dispersion independently of I'_p

$$\varepsilon(p) = \frac{K}{\pi} \sinh \gamma (1 - k^2 \cos^2 p)^{1/2}, \quad -\pi < p \leq 0 \quad (62)$$

(where the restriction on p follows from (50)), and the excited states can be regarded as states obtained by introducing excitations in one of the ground states, and the K_0 in (59) refers to the ground state in which the excitations are introduced.

Remember that for the two types of excitations the allowed values of Θ_h 's are different and the difference is of the order of $1/N$ (see (52)). Thus in the $N \rightarrow \infty$ limit not only the ground states become degenerate but the excitations above them, too.

6. Summary

In the present work we have studied the excitations of the anisotropic antiferromagnetic Heisenberg chain (1) for values of the anisotropy parameter $\rho > 1$. In this region the

ground state is doubly degenerated in the $N \rightarrow \infty$ limit and we have investigated the properties of the excitations above the two ground states. Our study is based on the Bethe ansatz equations (9) for the problem and we examined not only the density of the real roots but also the values of the roots themselves. The method used enables us to distinguish between the two types of ground states and excitations.

After rederiving the known result for the regular density of the real roots we eliminated these roots from the equations. The equations for the complex roots become slightly simpler as a consequence of our treatment (44). (In practice, the e^δ factor in equation (25) of *bv* has been evaluated and has been found to be equal to unity.) This means that the higher level equations have the same form for the whole antiferromagnetic region. Moreover we have given the equations for the parameters of the holes (52) and they show that the allowed values are different for the two types of excitations. (The difference is of the order of $1/N$.)

We have calculated the number of solutions for a given number of holes and complex roots; there are some identical solutions in the two groups of states but the 'overlapping' between the two groups vanishes in the $N \rightarrow \infty$ limit. The excitation energy has the same form for the two types of states so the corresponding states will become degenerate in the $N \rightarrow \infty$ limit.

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