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On the $S^z = 0$ excited states of an anisotropic Heisenberg chain

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Abstract. The $S^z = 0$ excited states of the anisotropic antiferromagnetic Heisenberg Hamiltonian

$$\hat{H} = \sum_{j=1}^{N} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \rho S_j^z S_{j+1}^z)$$

are studied when $0 \leq \rho \leq 1$. The original set of secular equations is reduced to a simpler one, which contains the parameters of excitations only. The energy–momentum dispersion is also found. It is shown that the typical low-lying excitations are either two-strings or not of string form. The simplest excitations are described in more detail.

1. Introduction

The study of exactly soluble models, like the 1D anisotropic Heisenberg model, has two-fold interest. First, such models provide non-trivial examples for interacting many-body systems, and this is in itself of great interest. The second point is, that although these models are very much simplified ones, their solutions can serve as checks for approximate methods used to solve more complicated but more realistic models.

In this work we study the low-energy excited states of the anisotropic Heisenberg Hamiltonian

$$\hat{H} = \sum_{j=1}^{N} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \rho S_j^z S_{j+1}^z) \tag{1.1}$$

where the spin operator with components S_j^x, S_j^y and S_j^z corresponds to an $S = \frac{1}{2}$ spin associated with the site j, and the problem is uniquely defined by the periodic boundary condition $S_{N+1} = S_1$.

The study of this Hamiltonian started a long time ago. The isotropic problem ($\rho = 1$) has already been investigated by Bethe (1931) and Hulten (1938). In particular Bethe could give a classification of the eigenstates of the isotropic Hamiltonian, and showed that finding the eigenvalues and eigenstates is equivalent to solving a set of coupled nonlinear equations. Orbach (1959) extended Bethe's treatment to the anisotropic case, and des Cloizeaux and Gaudin (1966) studied the ground state and the spin–wave states for all values of ρ. A strict mathematical proof of the uniqueness of the ground states for all values of ρ can be found in the papers by Yang and Yang (1966a, b, c) and the references for the $T = 0$ magnetic properties of the model are

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Griffiths (1964) and Yang and Yang (1966a, b, c). The lowest-energy excited states have been described by Johnson *et al* (1973). The thermodynamical properties of the model, following the work of Takahashi and Suzuki (1972), have been studied by Fowler and Zotos (1981, 1982) and Zotos and Fowler (1982).

Most of the work dealing with the 1D Heisenberg and related models has been based on some assumptions concerning the nature of the excited states. Our aim is to study these excited states, especially the $S^z = 0$ ones in the regime $0 \leqslant \rho < 1$. After introducing the general formalism (§ 2) in § 3 we reduce the original set of secular equations to a simpler system which contains the parameters of the excitations only. In § 4 the solutions of these equations for the two simplest cases are found.

2. Basic equations, the ground state, and notation

2.1. The basic equations

As is well known (Orbach 1959, des Cloizeaux and Gaudin 1966) according to Bethe's hypothesis, the $S^z = N/2 - r$ ($r \leqslant N/2$) eigenstates of (1.1) are given in the form

$$|\Omega\rangle = \sum_{n_1<n_2<\ldots<n_r} a(n_1, n_2, \ldots, n_r) S^-_{n_1} S^-_{n_2} \ldots S^-_{n_r} |F\rangle \tag{2.1}$$

where $S^-_{n_\alpha}$ flips down the spin at the site n_α, $|F\rangle$ is the ferromagnetic state with all spins pointing upwards, and the coefficients $a(n_1, n_2, \ldots, n_r)$ are

$$a(n_1, n_2, \ldots, n_r) = \sum_P \exp\left(\mathrm{i} \sum_{\alpha=1}^{r} k_{P\alpha} n_\alpha + \frac{\mathrm{i}}{2} \sum_{\alpha<\beta} \psi_{P\alpha P\beta}\right). \tag{2.2}$$

Here $(P1, P2, \ldots, P\alpha, \ldots, Pr)$ is a permutation of the numbers $(1, 2, \ldots, \alpha, \ldots, r)$ and the summation is extended over all permutations. Indeed, the state (2.1) with (2.2) represents an eigenstate of (1.1) with an energy measured from the energy of the state $|F\rangle$

$$E = \sum_{\alpha=1}^{r} (\cos k_\alpha - \rho) \tag{2.3}$$

if

$$\cot(\psi_{\alpha\beta}/2) = -\rho \frac{\cot(k_\alpha/2) - \cot(k_\beta/2)}{(1-\rho)\cot(k_\alpha/2)\cot(k_\beta/2) - (1+\rho)}. \tag{2.4}$$

Equation (2.4) together with the equations expressing the periodic boundary condition

$$N k_\alpha = 2\pi\lambda_\alpha + \sum_{\beta \neq \alpha} \psi_{\alpha\beta} \tag{2.5}$$

where all λ_α are integers are the equations to be solved for the complete description of the state classified by the quantum numbers $\lambda_1, \lambda_2, \ldots, \lambda_r$.

To make the system (2.4)–(2.5) simpler, auxiliary variables are introduced: in our case ($0 \leqslant \rho < 1$) the substitution (des Cloizeaux and Gaudin 1966)

$$\rho = \cos\Theta \qquad (0 < \Theta \leqslant \pi/2) \qquad \cot(k_\alpha/2) = \cot(\Theta/2)\tanh(\eta_\alpha/2) \tag{2.6}$$

is suitable. After this substitution $\psi_{\alpha\beta}$ depends on the difference $\eta_\alpha - \eta_\beta$ only and equations (2.4)–(2.5) can be written in the form

$$2N \tan^{-1}(\cot(\Theta/2) \tanh \eta_\alpha/2) = 2\pi \mathcal{F}_\alpha + \sum_{\beta=1}^{r} 2 \tan^{-1}[\cot \Theta \tanh(\eta_\alpha - \eta_\beta)/2]. \qquad (2.7)$$

Here the $\mathcal{F}_\alpha$ are integers if $N-r$ is odd and half odd-integers if $N-r$ is even ($\mathcal{F}_\alpha - (N-r-1)/2 = \text{integer}$). The energy of the state expressed in terms of these new variables is

$$E = -\sum_{\alpha=1}^{r} \frac{\sin^2 \Theta}{\cosh \eta_\alpha - \cos \Theta} \qquad (2.8)$$

and the momentum is

$$p = \sum_{\alpha=1}^{r} k_\alpha = -\frac{2\pi}{N} \sum_{\alpha=1}^{r} \mathcal{F}_\alpha + r\pi. \qquad (2.9)$$

2.2. *The ground state*

The ground state belongs to the $S^z = 0$ subspace if N is even and to the $S^z = \frac{1}{2}$ if N is odd. For the sake of simplicity we shall suppose that N is even. Then in order to describe the ground state one has to choose the $\mathcal{F}_\alpha$ set (des Cloizeaux and Gaudin 1966) as

$$\mathcal{F}_\alpha = -\tfrac{1}{2}(N/2 + 1 - 2\alpha) \qquad \alpha = 1, 2, \ldots, N/2. \qquad (2.10)$$

(This choice implies the conventions $0 < k_\alpha < 2\pi$, $-\pi < \psi_{\alpha\beta} < \pi$, $-\pi/2 < \tan^{-1} x < \pi/2$.)

With these quantum numbers all k_α (η_α) are real, and in the large N limit their density $\sigma_0(\eta)$ (the number of η_α in the interval $(\eta; \eta + \mathrm{d}\eta)$ is $N\sigma_0(\eta)\,\mathrm{d}\eta$) is

$$\sigma_0(\eta) = [4\Theta \cosh(\eta\pi/2\Theta)]^{-1}. \qquad (2.11)$$

The ground-state energy is

$$E_0 = -N \sin \Theta \int_0^\infty \left(1 - \frac{\tanh(\omega\Theta)}{\tanh(\omega\pi)}\right) \mathrm{d}\omega. \qquad (2.12)$$

2.3. *Extension to complex* η

It is interesting to note that in the ground state all k_α fall into the region $(\Theta; 2\pi - \Theta)$. It is very probable that the ground state is the only $S^z = 0$ state in which for all k_α

$$\operatorname{Im} k_\alpha = 0 \qquad \Theta < k_\alpha < 2\pi - \Theta. \qquad (2.13)$$

An argument supporting this is that in the planar limit ($\rho = 0$, $\Theta = \pi/2$) the only $S^z = 0$ state in which all k satisfy (2.13) is the ground state, thus supposing continuity in Θ one has to assume that in the excited states, (2.13) does not hold for all k_α.

Since (2.6) defines real η for k satisfying (2.13) only, (2.6) must also be extended to complex variables. In doing this, we shall use the definitions

$$\begin{aligned}2 \tan^{-1}[\cot \Theta \tanh(\varphi + \mathrm{i}\chi)] &= \{2 \tan^{-1}[\cot \Theta \tanh(\varphi + \mathrm{i}\chi)]\}_{\text{cont}} \\ &\quad + \{2 \tan^{-1}[\cot \Theta \tanh(\varphi + \mathrm{i}\chi)]\}_{\text{discont}} \qquad (2.14a)\end{aligned}$$

$$\{2\tan^{-1}[\cot\Theta\tanh(\varphi+i\chi)]\}_{\rm cont}$$
$$=\frac{1}{2i}\ln\frac{\cosh 2\varphi-\cos 2(\Theta-\chi)}{\cosh 2\varphi-\cos 2(\Theta+\chi)}+\tan^{-1}[\cot(\Theta-\chi)\tanh\varphi]$$
$$+\tan^{-1}[\cot(\Theta+\chi)\tanh\varphi] \qquad (2.14b)$$

$$\{2\tan^{-1}[\cot\Theta\tanh(\varphi+i\chi)]\}_{\rm discont}$$
$$=(\pi/2)(\operatorname{sgn}\varphi)[\operatorname{sgn}(\chi-\Theta)+\operatorname{sgn}(\chi-\Theta+\pi)+\operatorname{sgn}(-\chi-\Theta)$$
$$+\operatorname{sgn}(-\chi-\Theta+\pi)]. \qquad (2.14c)$$

(Here we understand that $0<\Theta<\pi$, $-\pi<\chi\leqslant\pi$ and $|\tan^{-1}\chi|\leqslant\pi/2$ for real χ.)

It is easy to see that complex k define complex η with $|\mathrm{Im}\,\eta|<\pi$ while real k not falling in the region $(\Theta; 2\pi-\Theta)$ correspond to complex η with $\mathrm{Im}\,\eta=\pi$. As in any $S^z=0$ excited state some of the k are supposed not to satisfy (2.13), in order to find $S^z=0$ excitations one has to look for those solutions of equation (2.7) in which some of the η are complex with $-\pi<\mathrm{Im}\,\eta\leqslant\pi$. A usual way of treating states with complex η is to suppose that the complex η are arranged in special configurations (the so-called strings) of the form

$$\eta^{nk}_{\alpha\nu}=\eta^{n}_{\alpha}+i(n+1-2k)\Theta+i(\pi/2)(1-\nu)+O(\exp(-N)) \qquad (2.15)$$

(with η^n_α being real, ν can be + or -1, and $k=1,2,\ldots,n$) and to deduce equations for the centres of the strings i.e. for the η^n_α. Now we follow a different strategy: we do not make assumptions on the forms of the complex variables; instead we eliminate the real η from equation (2.7) to obtain a system which contains the parameters of the excitations i.e. the complex η-set and the positions of the holes left behind in the real η distribution only. We shall find that the complex η need not be of string form, moreover in the typical low-energy excited states the complex η do not form longer than two-strings. Instead of the longer strings, other non string-type complex η configurations can appear.

3. Equations for the states with several complex η

In this section we shall derive equations for the parameters characteristic for the states with complex η. The complex η will be labelled by Latin indices n and m to distinguish them from the real η labelled by Greek indices. The real and imaginary parts of the η_n will be denoted by φ_n and χ_n respectively: $\eta_n=\varphi_n+i\chi_n$. The numbers $2n_1$, $2n_2$ and n_3 will denote the numbers of complex η with $|\chi|<2\Theta$, $2\Theta<|\chi|<\pi$ and $\chi=\pi$, respectively. The total number of η is $r=N/2$.

3.1. Density of the real η

It is convenient to write equation (2.7) for the real η in the form

$$N2\tan^{-1}[\cot(\Theta/2)\tanh(\eta_\alpha/2)]$$
$$=2\pi\mathscr{F}'_\alpha+\sum_\beta 2\tan^{-1}[\cot\Theta\tanh(\eta_\alpha-\eta_\beta)/2]$$
$$+\sum_n\{2\tan^{-1}[\cot\Theta\tanh(\eta_\alpha-\eta_n)/2]\}_{\rm cont} \qquad (3.1)$$

where we introduced

$$\mathscr{F}'_\alpha = \mathscr{F}_\alpha + \frac{1}{2\pi}\sum_n \{2\tan^{-1}[\cot\Theta \tanh(\eta_\alpha - \eta_n)/2]\}_{\text{discont}}. \tag{3.2}$$

The parity of the numbers $2\mathscr{F}'_\alpha$ is the same as that of the number $N/2 - n_3 - 1$. It is not hard to show that equation (3.1) has a solution if all $\mathscr{F}'_\alpha$ are different and $|\mathscr{F}'_\alpha| < \frac{1}{2}(N/2 + 2n_2 + n_3)$. (The same proof can be adopted here which was used by Griffiths (1964) to show the existence of a solution for equations (2.4)–(2.5) for a λ set: $0 < \lambda_\alpha$, $\lambda_\alpha + 2 \leqslant \lambda_{\alpha+1} < N$.) Also taking into account the restriction on the parities of the $2\mathscr{F}'_\alpha$ we find that for the $\mathscr{F}'_\alpha$ set we have to choose $N/2 - 2n_1 - 2n_2 - n_3$ different numbers from the set

$$-\tfrac{1}{2}(N/2 + 2n_2 + n_3 - 1), -\tfrac{1}{2}(N/2 + 2n_2 + n_3 - 3), \ldots, \tfrac{1}{2}(N/2 + 2n_2 + n_3 - 1). \tag{3.3}$$

Equation (3.1) defines real η (later on denoted by η_h) also for the $2n_1 + 4n_2 + 2n_3 = H$ numbers left out of the set (3.3) (denoted by $\mathscr{F}'_h$)

$$N2\tan^{-1}(\cot(\Theta/2)\tanh\eta_h/2) = 2\pi\mathscr{F}'_h + \sum_\beta 2\tan^{-1}[\cot\Theta\tanh(\eta_h - \eta_\beta)/2]$$
$$+ \sum_n \{2\tan^{-1}[\cot\Theta\tanh(\eta_h - \eta_n)/2]\}_{\text{cont}}. \tag{3.4}$$

In the large-N limit with the above choice of $\mathscr{F}'_\alpha$ equation (3.1) can be turned by standard methods into a linear integral equation for the density of η_α, which, when solved by Fourier transformation, yields

$$\sigma(\eta) = \sigma_0(\eta) + \frac{1}{N}\sigma_1(\eta) + \frac{1}{N}\sigma_2(\eta) \tag{3.5}$$

where $\sigma_0(\eta)$ is the ground-state density given by (2.11); $\sigma_1(\eta)$ and $\sigma_2(\eta)$ the contributions corresponding to the presence of the η_h and η_n respectively are

$$\sigma_1(\eta) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left(-\frac{\sinh\omega\pi}{2\sinh\omega(\pi-\Theta)\cosh\omega\Theta}\right)\sum_h \exp[\mathrm{i}\omega(\eta - \eta_h)]\,\mathrm{d}\omega \tag{3.6}$$

$$\sigma_2(\eta) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\sum_n\left(-\frac{f(\omega, 2\Theta, -\chi_n)}{2\sinh\omega(\pi-\Theta)\cosh\omega\Theta}\right)\exp[\mathrm{i}\omega(\eta - \varphi_n)]\,\mathrm{d}\omega. \tag{3.7}$$

The function $f(\omega, \Theta, \chi)$ is defined as

$$f(\omega, \Theta, \chi) = \sinh\omega\pi\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega\varphi}\frac{\sin\Theta}{\cosh(\varphi + \mathrm{i}\chi) - \cos\Theta}\,\mathrm{d}\varphi. \tag{3.8}$$

We note here that $\sigma(\eta)$ of (3.5) can be regarded as the density of η_α only if $\sigma(\eta) + (1/N)\sum_h \delta(\eta - \eta_h)$ is positive for all η. This is true if the number of complex η is small compared with N (in this case $\sigma(\eta)$ is dominated by $\sigma_0(\eta)$) but is not obvious if H is comparable to N (in which case $\sigma_2(\eta)$ may make $\sigma(\eta)$ negative). For this, for large H the positiveness of $\sigma(\eta) + (1/N)\sum_h \delta(\eta - \eta_h)$ must be checked for any given solution.

3.2. Equations for the complex η

Equation (2.7) for a complex η takes the form

$$N2\tan^{-1}(\cot(\Theta/2)\tanh\eta_n/2) = 2\pi\mathcal{F}_n + \sum_\beta 2\tan^{-1}[\cot\Theta\tanh(\eta_n-\eta_\beta)/2] + \sum_m 2\tan^{-1}[\cot\Theta\tanh(\eta_n-\eta_m)/2]. \tag{3.9}$$

Replacing the continuous part of the sum over the real η by an integral over the real η with density (3.5) after some algebra we get

$$\left.\begin{array}{ll} N2\tan^{-1}[\tanh(\eta_n\pi/4\Theta)] & \text{if } |\chi_n|<2\Theta \\ N\pi\,\mathrm{sgn}\,\varphi_n & \text{if } |\chi_n|>2\Theta \end{array}\right\} = 2\pi\mathcal{F}_n + \sum_\beta \{2\tan^{-1}[\cot\Theta\tanh(\eta_n-\eta_\beta)/2]\}_{\text{discont}} + \sum_m 2\tan^{-1}[\cot\Theta\tanh(\eta_n-\eta_m)/2] + \int_{-\infty}^{\infty}\{2\tan^{-1}[\cot\Theta\tanh(\eta_n-\eta')/2]\}_{\text{cont}}(\sigma_1(\eta')+\sigma_2(\eta'))\,d\eta'. \tag{3.10}$$

What is interesting in this equation is that the imaginary part of the LHS is proportional to N if $|\chi_n|<2\Theta$ but it is zero if $2\Theta<|\chi_n|\leqslant\pi$. This means that in the first case equation (3.10) can only be satisfied if at the same time the RHS has an imaginary part of the order of N, that is, for an η_n with $|\chi_n|<2\Theta$ there is another $\eta_{n'}$ for which

$$2\tan^{-1}[\cot\Theta\tanh(\eta_n-\eta_{n'})/2]\sim N \tag{3.11}$$

i.e. (see equation (2.14*b*))

$$\eta_n-\eta_{n'}=\pm i2\Theta\pm 2\delta \tag{3.12}$$

with $|\delta|$ being exponentially small in N. As the term (3.11) also appears on the RHS of equation (3.10) for the $\eta_{n'}$ (with a minus sign) it is also clear that $|\chi_{n'}|<2\Theta$. Thus we conclude that the set of complex η_n with $|\chi_n|<2\Theta$ must consist of pairs satisfying (3.12), that is pairs of the form

$$\eta_n^+=\varphi_n+i(\mu_n+\Theta)+\delta_n \qquad \eta_n^-=\varphi_n+i(\mu_n-\Theta)-\delta_n \qquad |\mu_n|<\Theta. \tag{3.13}$$

In connection with the above reasoning we have to note the following. One point is that equation (3.10) requires only that the η_n with $|\chi_n|<2\Theta$ have a partner with which (3.12) is satisfied, but does not impose restrictions on the forms of η_n with $|\chi_n|>2\Theta$. The other point is that if in (3.13) $\mu_n=0$, η_n^+ and η_n^- are the complex conjugates of each other ($\mathrm{Re}\,\delta_n=0$) and they represent an ordinary two-string. If however $\mu_n\neq 0$, the $\eta_n^\pm$ pair should be regarded as a two-string with a complex centre. Since each η_n should appear together with its complex conjugate (except for $\chi_n=\pi$) if $\mu_n\neq 0$ there must be another $\eta_{n'}^\pm$ pair which has its centre at $\varphi_n-i\mu_n$ and the two $\eta_n^\pm$ pairs form a quartet of the form

$$\begin{array}{ll} \eta_n^+=\varphi_n+i(\mu_n+\Theta)+\delta_n & \eta_n^-=\varphi_n+i(\mu_n-\Theta)-\delta_n \\ \eta_{n'}^+=\varphi_n+i(-\mu_n+\Theta)-\delta_n^* & \eta_{n'}^-=\varphi_n+i(-\mu_n-\Theta)+\delta_n^*. \end{array} \tag{3.14}$$

Later on it will be convenient to represent the η_n set by a set of auxiliary variables ψ_n which are defined as follows.

(i) One complex η pair $\eta_n^{\pm}$ of the form of (3.13) is represented by a single ψ_n:

$$\psi_n = \varphi_n + \mathrm{i}\mu_n \qquad |\mu_n| < \Theta. \tag{3.15}$$

(ii) A complex η_n with $|\chi_n| > 2\Theta$ is represented by a ψ_n of the form

$$\psi_n = \varphi_n + \mathrm{i}\mu_n \qquad \mu_n = \chi_n - \Theta \operatorname{sgn} \chi_n \qquad \Theta < |\chi_n| \leq \pi - \Theta. \tag{3.16}$$

The ψ_n set consists of real numbers, complex conjugate pairs with $0 < |\mathrm{Im}\, \psi_n| < \pi - \Theta$ and complex numbers with $\mathrm{Im}\, \psi_n = \pi - \Theta$. The total number of the ψ_n is $n_1 + 2n_2 + n_3 = H/2$, that is half of the number of holes in the real η distribution.

The equation for a ψ_n with $|\mu_n| < \Theta$ can be obtained by summing up equation (3.10) for the corresponding η_n^+ and η_n^-. Doing so, the large terms of the two equations cancel each other and in the remaining part the δ can be neglected (see also the appendix). The equations for the ψ_n with $|\mu_n| > 2\Theta$ are obtained simply by rearranging the terms in equation (3.13) for the corresponding η_n and neglecting the exponentially small δ. As a result, we get for all ψ_n

$$\sum_{h=1}^{H} 2 \tan^{-1}[\cot(\Theta'/2) \tanh(\psi_n' - \eta_h')/2]$$
$$= 2\pi \mathscr{F}_n' + \sum_{m=1}^{H/2} 2 \tan^{-1}[\cot \Theta' \tanh(\psi_n' - \psi_m')/2]. \tag{3.17}$$

Here we used the notations

$$\Theta' = \frac{\pi}{\pi - \Theta}\Theta \qquad \eta_h' = \frac{\pi}{\pi - \Theta}\eta_h \qquad \psi_n' = \frac{\pi}{\pi - \Theta}\psi_n = \varphi_n' + \mathrm{i}\mu_n'. \tag{3.18}$$

The $\mathscr{F}_n'$ parameters are obtained by collecting the terms of the form $n\pi$. Their connections with the original $\mathscr{F}_n$ are

$$\mathscr{F}_n' = \mathscr{F}_n^+ + \mathscr{F}_n^- - \tfrac{1}{2}N \operatorname{sgn} \varphi_n + \tfrac{1}{2} \sum_{m \neq n} \operatorname{sgn}(\varphi_n - \varphi_m) \qquad \text{if } |\mu_n'| < \Theta'$$
$$\mathscr{F}_n' = \mathscr{F}_n - \tfrac{1}{2}N \operatorname{sgn} \varphi_n + \tfrac{1}{2} \sum_{\beta} \operatorname{sgn}(\varphi_n - \eta_\beta) + \tfrac{1}{2} \sum_{h} \operatorname{sgn}(\varphi_n - \eta_h)$$
$$+ \tfrac{1}{2} \sum_{|\mu_m'| < \Theta'} \operatorname{sgn}(\varphi_n - \varphi_m) \qquad \text{if } |\mu_n'| > \Theta'. \tag{3.19}$$

The parity of the numbers $2\mathscr{F}_n'$ is the same as that of $H/2 - 1$.

3.3. *Equations for the variables η_h*

The equation for the η_h is obtained from equation (3.4) by replacing the sum over the η_β on the RHS by an integral over the η with density $\sigma(\eta)$. This way one gets

$$N 2 \tan^{-1}[\tanh(\eta_h' \pi / 4\Theta')] = 2\pi \mathscr{F}_h'' - \sum_{h'} \phi(\eta_h' - \eta_{h'}')$$
$$+ \sum_{n} 2 \tan^{-1}[\cot(\Theta'/2) \tanh(\eta_h' - \psi_n')/2] \tag{3.20}$$

where

$$\phi(x)=\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\mathrm{i}\omega}\frac{\sinh\omega(\pi-\Theta')}{2\sinh\omega\pi\cosh\omega\Theta'}\mathrm{e}^{\mathrm{i}\omega x} \tag{3.21}$$

and

$$\mathscr{F}''_h=\mathscr{F}'_h-\frac{1}{2\pi}\sum_n\{2\tan^{-1}[\cot(\Theta'/2)\tanh(\eta'_h-\psi'_n)/2]\}_{\text{discont}}. \tag{3.22}$$

The $\mathscr{F}''_h$ parameters are integers if $N/2$ is odd and half odd-integers if $N/2$ is even.

3.4. Remarks in connection with the system (3.17), (3.20)

By solving the system (3.17) and (3.20) one can construct the solution of the original equation (2.7): if the ψ_n are given according to (3.13), (3.15)–(3.16) the complex η can be calculated (up to exponentially small terms) and knowing also the η_h through equations (3.5)–(3.7) the density of η_α can be determined too. The η set obtained this way satisfies equation (2.7) if both the δ_n are small (see appendix) and the $\sigma(\eta)+(1/N)\Sigma_h\,\delta(\eta-\eta_h)$ is positive (see the paragraph after (3.8)).

The system (3.17), (3.20) can also be used to calculate the excited states of an isotropic ($\rho=1$) Heisenberg chain simply by taking the $\Theta\to 0$ limit. In this limit all η (except those with $\mathrm{Im}\,\eta=\pi$) disappear proportionally to Θ while the η/Θ ($\to\cot(k/2)$) ratios remain finite From the complex η with $\mathrm{Im}\,\eta=\pi$ only the 'discont' parts of the $\tan^{-1}$ functions remain. It is not hard to check that this procedure leads to the same equations as the procedure described in §§ 3.1–3.3 applied directly on the secular equations of the isotropic Heisenberg chain.

As has been mentioned in § 2 the usual approach to describe states with complex wavenumbers is to look for string solutions (see (2.15)). It is not hard to see that the ψ'_n parameters representing the η_n-set of a string should also form a string (but a shorter one and with a spacing in the imaginary direction $2\Theta'$). Equation (3.17), however, has string solutions only if H is sufficiently large. Otherwise there is no reason for having terms with large imaginary parts on the RHS and there is no restriction on the imaginary parts of the ψ'_n. Thus the typical complex η configurations for small H are the ordinary two-strings (real ψ_n), quartets of the form $\varphi_n\pm\mathrm{i}(\mu_n\pm\Theta)$ ($|\mathrm{Im}\,\psi'_n|<\Theta'$) complex η pairs with $|\mathrm{Im}\,\eta_n|>2\Theta$ ($|\mathrm{Im}\,\psi'_n|>\Theta'$) and complex η_n with $\mathrm{Im}\,\eta_n=\pi$ ($\mathrm{Im}\,\psi_n=\pi$). It is also worth noting that changing the positions of the η_h one of these complex η configurations can go over into another one continuously, thus we cannot prefix the positions of the holes in the real η distribution and the types of the complex η configurations independently.

The results concerning the complex η not forming strings seem to be in contradiction with the findings of Fowler and Zotos (1981) and Hida (1981). In both papers it is argued that the normalisability of the wavefunction requires the complex η to form strings. In principle, in both papers the arguments concerned infinitely long chains with a finite number of turned down spins. Now we are dealing with long but finite chains with a periodic boundary condition which is built in in equation (2.7). Thus all the solutions of equation (2.7) should give normalisable wavefunctions.

3.5. Energy and momentum of the states with complex η

The energy is calculated according to the formula (2.8). Evaluating the contribution of the real η by means of $\sigma(\eta)$ it turns out that the contribution of the complex η

drops out and only the contribution of the holes remains

$$E = E_0 + \frac{\pi}{2}\frac{\sin\Theta}{\Theta}\sum_h \frac{1}{\cosh(\eta_h\pi/2\Theta)}. \tag{3.23}$$

The momentum using (2.9), (3.2), (3.3), (3.17), (3.19), (3.20) and (3.22) is

$$p = -\sum_h p_h + \sum_n \pi(1 - \operatorname{sgn}\varphi_n) + \tfrac{1}{2}N\pi \tag{3.24}$$

with

$$0 < p_h = \tfrac{1}{2}\pi - 2\tan^{-1}[\tanh(\eta_h\pi/4\Theta)] < \pi \tag{3.25}$$

which compared with (3.23) yields

$$E - E_0 = \sum_h \frac{\pi}{2}\frac{\sin\Theta}{\Theta}\sin p_h \qquad p - p_0 = \sum_h -p_h \ (\text{mod } 2\pi). \tag{3.26}$$

The fact that the energy–momentum dispersion contains explicitly only the positions of the holes in the real η distribution suggests that these states should be classified according to the number of holes, rather than according to the number of complex η. This is in accordance with the fact that at fixed H changing the positions of η_h may cause changes in the number of η_n (one $|\text{Im}\,\psi'|$ crossing Θ' changes the number of η_n by two).

4. The simplest excited states

4.1. States with two holes in the real η distribution

For $H = 2$ there is only one ψ'. For this, $\text{Im}\,\psi'$ is either zero or π. In both cases equation (3.17) (with $\mathcal{F}' = 0$) yields

$$\text{Re}\,\psi' = (\eta'_{h_1} + \eta'_{h_2})/2 = \varphi'. \tag{4.1}$$

If $\text{Im}\,\psi' = 0$, (4.1) corresponds to a complex η and k pair

$$\begin{aligned} \eta^{\pm} &= \tfrac{1}{2}(\eta_{h_1} + \eta_{h_2}) \pm \mathrm{i}\Theta \\ k^{\pm} &= \tfrac{1}{2}\pi(2 - \operatorname{sgn}\varphi) - \tan^{-1}(\cot\Theta\tanh\varphi/2) \pm \frac{\mathrm{i}}{2}\ln\frac{\cosh\varphi - 1}{\cosh\varphi - \cos 2\Theta} \end{aligned} \tag{4.2}$$

while for $\text{Im}\,\psi' = \pi$ the corresponding complex η and real k are

$$\eta = \tfrac{1}{2}(\eta_{h_1} + \eta_{h_2}) + \mathrm{i}\pi \qquad k = \pi(1 - \operatorname{sgn}\varphi) - \tan^{-1}(\tan(\Theta/2)\cdot\tanh\varphi/2). \tag{4.3}$$

With $\text{Re}\,\psi'$ given by (4.1), equation (3.20) can be solved numerically for η_{h_1} and η_{h_2} if $\mathcal{F}''_{h_1}$ and $\mathcal{F}''_{h_2}$ are two different ($\text{Im}\,\psi' = 0$) or two different or equal ($\text{Im}\,\psi' = \pi$) numbers between $\pm(N/2)(N/2-1)$. The numbers of different solutions are $(N/2)\times(N/2-1)/2$ and $(N/2)(N/2+1)/2$, respectively. Both classes of the above states have an energy–momentum dispersion

$$E = E_0 = \tfrac{1}{2}\pi(\sin\Theta/\Theta)(\sin p_{h_1} + \sin p_{h_2}). \tag{4.4}$$

The solutions of equation (3.17) described above correspond to the lowest-energy $S^z = 0$ excited states described by Johnson *et al* (1973). It is worth noting that taking the $\rho \to 1$ ($\Theta \to 0$) isotropic limit, the states corresponding to (4.2) go over into the singlet states with one complex k pair, while the limiting states corresponding to (4.3) are the simplest $S^z = 0$ triplet states (Yamada 1969). In the $\rho \to 0$ ($\Theta \to \pi/2$) planar limit the states characterised by p_1 and p_2 of both classes go over into different linear combinations of the states which are obtained by filling in all modes between $\pi/2$ and $3\pi/2$, and exciting one particle from the mode $\pi/2 + p_1$ to $\pi/2 - p_2$ and vice versa. This solves the apparent contradiction, that Im $k^{\pm}$ in (4.2) does not vanish even if the 'interaction part' from the Hamiltonian is absent.

4.2. *The states with four holes in the real η distribution*

For $H = 4$ the number of ψ' is two. Although equation (3.17) can also be solved analytically in this case, since the results are less transparent, we just give an account of the different solutions. To any given set of the four η_h, equation (3.17) has six different solutions which generate solutions for equation (2.7), and these solutions can be grouped into the following four classes:

(i) a real ψ' pair;

(ii) three different ψ' pairs; in each pair one Im ψ' is zero, the other is π;

(iii) a ψ' pair, with both Im $\psi' = \pi$;

(iv) a ψ' pair, which, depending on the actual values of the η_h, can either be real or complex and for which $0 \leqslant |\text{Im}\ \psi'| < \pi/2$ if $\Theta' < \pi/2$, and $\pi/2 < |\text{Im}\ \psi'| \leqslant \pi$ if $\pi/2 < \Theta' \leqslant \pi$.

In all four classes the ψ' are continuous functions of the η_h. Solutions belonging to the first three classes generate states with two two-strings, states with one two-string and a real k outside $(\Theta; 2\pi - \Theta)$, and states with two real k outside $(\Theta; 2\pi - \Theta)$, respectively. The states belonging to class (iv) appeared instead of the states with one three-string (also a three-string would require four holes in the real η distribution), and depending on the four momenta (η_h) they can be states with either two two-strings or with one quartet (see (3.14)) or with a single complex k pair not forming a two-string if $\Theta < \pi/3$, and they can be states with either one quartet or with a complex k pair not forming a two-string, or states with two real k outside the interval $(\Theta; 2\pi - \Theta)$ if $\pi/3 < \Theta < \pi/2$. For all four classes the energy–momentum dispersion is

$$E - E_0 = \sum_{h=1}^{4} \frac{\pi}{2} \frac{\sin \Theta}{\Theta} \sin p_h \tag{4.5}$$

thus (4.5) is six-fold degenerated.

In the $\rho \to 1$ isotropic limit the states of classes (i) and (iv) go over into singlet ones, while the states belonging to classes (ii) and (iii) are $S^z = 0$ triplet and $S^z = 0$, $S^2 = 6$ ones respectively. In the planar limit the states of all four classes go over into (two-particles, two-holes)-like states.

5. Summary

In the present work we have studied the $S^z = 0$ excited states of the anisotropic antiferromagnetic Heisenberg chain for values of the anisotropy parameter $0 \leqslant \rho \leqslant 1$. Our study has been based on the secular equations for the problem (equation (2.7)).

It has been argued that to describe the $S^z = 0$ excitations complex η parameters should be introduced. From the original equation (2.7) a simpler system (equations (2.17), (3.20)) has been deduced. This system contains only the variables characteristic for the excitations: a set of auxiliary variables which represents the set of complex η and the positions of the holes in the real η distribution. The energy–momentum dispersion is also determined. It does not depend explicitly on the number and the distribution of the complex η but the positions of the holes: $p = \Sigma_h (-p_h)$; $E - E_0 = \Sigma_h (\pi/2)(\sin \Theta/\Theta) \sin p_h$, where the p_h momenta are determined by the holes only (equation (3.25)).

It has been a general opinion, that the complex η obtainable as solutions of the secular equations (2.7) should form strings. A simple argument based on the form of equation (3.17) shows, however, that string solutions, except the two-string ones, can exist only if the number of holes in the real η distribution is sufficiently large. If the number of holes is small, longer strings do not exist, and the typical complex η configurations are the two-strings, quartets of the form $\varphi \pm i\mu \pm i\Theta$ ($|\mu| < \Theta$), complex η pairs with $|\mathrm{Im}\, \eta| > 2\Theta$ and complex η with $\mathrm{Im}\, \eta = \pi$.

Solutions of equations (3.17), (3.20) for the simplest excited states are described. If the number of holes is two, two classes of solutions exist. The first corresponds to states with one two-string, while the second corresponds to states with one real k outside $(\Theta; 2\pi - \Theta)$. The excited states with four holes in the real η distribution can be grouped into four classes: the first three classes are given by the states with two two-strings, one two-string and one real k outside $(\Theta; 2\pi - \Theta)$, and two real k outside $(\Theta; 2\pi - \Theta)$, respectively. States falling into the fourth class are, depending on the momenta, states with either two two-strings, or one quartet, or a complex k pair not forming a two-string, or states with two real k not falling in the region $(\Theta; 2\pi - \Theta)$. The energy–momentum dispersion for the states with two holes are two-fold, while for the states with four holes are six-fold degenerated.

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Appendix. Equations for the δ

When deriving equations for the ψ_n the δ_n (see (3.13)) have been neglected. Thus the consistency of the whole treatment requires that the δ_n are indeed small. This can be checked after writing the equations for the δ_n.

Taking equation (3.10) for η_n^+ and η_n^- and subtracting one from the other leads to the equation

$$\begin{aligned} &2N[\![\tan^{-1}\{\tanh[\tfrac{1}{2}(\psi_n + i\Theta)\pi/2\Theta]\} - \tan^{-1}\{\tanh[\tfrac{1}{2}(\psi_n - i\Theta)\pi/2\Theta]\}]\!] - 2\pi(\mathscr{F}_n^+ - \mathscr{F}_n^-) \\ &\quad - \sum_h \int_{-\infty}^{\infty} \frac{\sinh \omega(\pi - 2\Theta) \sinh \omega\Theta}{\sinh \omega(\pi - \Theta) \cosh \omega\Theta} \exp[i\omega(\psi_n - \eta_h)] \frac{d\omega}{i\omega} \\ &\quad + \sum_{m \neq n} 2\{\tan^{-1}[\cot(\Theta'/2) \tanh \tfrac{1}{2}(\psi'_n - \psi'_m - i\Theta')] \\ &\quad - \tan^{-1}[\cot(\Theta'/2) \tanh \tfrac{1}{2}(\psi'_n - \psi'_m + i\Theta')]\} \\ &\quad + 2\int_{-\infty}^{\infty} \frac{\sinh^2 \omega(\pi - 2\Theta) \sinh \omega\Theta}{\sinh \omega\pi \sinh \omega(\pi - \Theta)} \frac{d\omega}{i\omega} \\ &\quad = 4 \tan^{-1}[\cot \Theta \tanh(i\Theta + \delta_n)]. \end{aligned} \tag{A1}$$

If the ψ_n (ψ'_n) and η_h are given, with an appropriate choice of the number $\mathscr{F}_n^+ - \mathscr{F}_n^-$ (A1) can be solved for δ_n. Note, that for the sake of consistency, the parity of the number $\mathscr{F}_n^+ - \mathscr{F}_n^-$ must be the same as that of $N/2 - 1 + \mathscr{F}_n^+ + \mathscr{F}_n^-$. With this restriction both the choice of $\mathscr{F}_n^+ - \mathscr{F}_n^-$ and the solution for δ_n is unique.

The modulus of δ_n is determined by the imaginary part of equation (A1). If we have a small number of excitations ($H \ll N$) then the imaginary part of the LHS is dominated by that of the first term, which is negative and proportional to N, meaning that $|\delta_n|$ is indeed exponentially small in N. If, however, H is comparable to N, the other terms can also contribute significantly. In this case the smallness of the δ_n must be checked for each solution of equations (3.17), (3.20).

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