KFKI-1981-70

F. WOYNAROVICH

ON THE $S^z=0$ EXCITED STATES OF AN ANISOTROPIC HEISENBERG CHAIN

Hungarian Academy of Sciences

CENTRAL RESEARCH INSTITUTE FOR PHYSICS

BUDAPEST

KFKI-1981-70

ON THE $S^z=0$ EXCITED STATES OF AN ANISOTROPIC HEISENBERG CHAIN

F. Woynarovich

Central Research Institute for Physics
H-1525 Budapest 114, P.O.B. 49, Hungary

HU ISSN 0368 5330
ISBN 963 371 852 X

ABSTRACT

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

$$\hat{H} = \sum_{j=1}^{N} (S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \rho S^z_j S^z_{j+1})$$

are studied in the case $0 \leq \rho \leq 1$. The original set of secular equations is reduced to a simpler one, which contains only the parameters of the excitations. The energy-momentum dispersion of the excitations is also found. The simplest excitations are described and studied in more detail. It is found that they can be groupped into two classes, one of them corresponding to the simplest singlet, the other corresponding to the simplest triplet excitations in the isotropic limit.

АННОТАЦИЯ

Исследованы $S^z=0$ возбужденные состояния одномерного, анизотропного, ферромагнитного гейзенберговского гамильтониана

$$\hat{H} = \sum_{j=1}^{N} (S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \rho S^z_j S^z_{j+1})$$

в случае $0 \leq \rho \leq 1$. Из системы секулярных уравнений задачи получена более простая система, содержащая только параметры возбуждений. Определен закон дисперсии возбуждений. Простейшие возбуждения более детально изучены и показано, что они могут быть разделены на два класса. Принадлежащие к первому классу возбуждения соответствуют простейшим синглетным возбуждениям в изотропном пределе, а классифицированные во второй класс соответствуют простейшим триплетным возбуждениям в том же пределе.

KIVONAT

A $\hat{H} = \sum_{j=1}^{N} (S^x_j S^x_{j+1} + S^y_j S^y_{j+1} + \rho S^z_j S^z_{j+1})$ 1-d anisotrop antiferromágneses Heisenberg Hamilton operátor $S^z=0$ gerjesztett állapotait vizsgáljuk $0 \leq \rho \leq 1$ mellett. Az eredeti szekuláris egyenletrendszerből egy olyan egyszerübb egyenletrendszert származtatunk, amely már csak a gerjesztések paramétereit tartalmazza. Meghatározzuk a gerjesztések energia-impulzus diszperzióját is. A legegyszerübb gerjesztéseket részletesebben is megvizsgáljuk. Azt találjuk, hogy ezek két osztályba sorolhatóak, az egyik osztályba tartozóak a legegyszerübb singlet, a másik osztályba tartozóak pedig a legegyszerübb triplet gerjesztéseknek felelnek meg az izotrop határesetben.

1. INTRODUCTION

The study of exactly soluble models, like the 1-d anisotropic Heisenberg model, has twofold interest. First, such models provide nontrivial 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

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

where the spin operator with components S_j^x, S_j^y and S_j^z corresponds to an $S = 1/2$ 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 ($\rho = 1$) was already 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 non-linear equations. He succeeded in calculating the ground-state energy, too. Des Cloizeaux and Pearson (1962) determined a class of excited states, the so called spin-wave states. Orbach (1959) extended Bethe's treatment to the anisotropic case and Walker (1959) gave an analitical expression for the ground state energy for $\varrho \geq 1$. 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-state for all values of ϱ can be found in the papers by Yang and Yang (1966); and the references for the $T=0$ magnetic properties of the model are: Griffiths (1964) and Yang and Yang (1966).

Our aim is to study the $S^z=0$ excited states in the region $0 \leq \varrho < 1$. In Section 2. after introducing the general formalism we argue, that the states in question should be described by complex parameters. In Section 3. from the original set of secular equations (see for eg. des Cloizeaux and Gaudin (1966)) a simpler system is deduced which contains the parameters of the excitations only. In Section 4. the solutions of these equations for the two simplest case are found: those two classes of states are identified , which go over to the simplest singlet and simplest triplet spin wave states in the $\varrho \to 1$ isotropic limit.

2. BASIC EQUATIONS, GROUND STATE, NOTATIONS

2.1 The basic equations

As it is known (Orbach (1959) des Cloizeaux, Gaudin (1966)) according to Bethe's hypothesis, the eigenstates of (1.1) with $r\,(\leq N/2)$ reversed spins can be given in the form

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

where $S^-_{n_i}$ flips down the spin at the site n_i ; $|F\rangle$ is the ferromagnetic state with all spins pointing upwards, and the coefficients $a(n_1,n_2,\dots n_r)$ are given in the form

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

Here $(P1, P2, \dots, P\alpha, \dots, Pr)$ is a permutation of the numbers $(1, 2, \dots, \alpha, \dots, r)$, and the summation is extended over all permutations. The expression in (2.1) with the coefficients given in (2.2) represents indeed 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

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

Eq. (2.4) together with the equations expressing the periodic boundary conditions

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

with all λ_α being integers, are the equations to be solved for the complet 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 $(0 \leq \rho < 1)$ the substitution (des Cloizeaux and Gaudin (1966))

$$\rho = \cos\Theta$$
$$\cot(k_\alpha/2) = \cot(\Theta/2).\tanh(\eta_\alpha/2) \tag{2.6a}$$

is suitable. With this

$$\cot(\psi_{\alpha\beta}/2) = \cot\Theta\tanh((\eta_\alpha - \eta_\beta)/2) \tag{2.6b}$$

Thus (2.4) and (2.5) take the form

$$N2\,\mathrm{arccot}\left(\cot\frac{\Theta}{2}\tanh\frac{\eta_\alpha}{2}\right) = 2\pi\lambda_\alpha + \sum_{\beta\neq\alpha} 2\,\mathrm{arccot}\left(\cot\Theta\tanh\frac{\eta_\alpha-\eta_\beta}{2}\right) \tag{2.7a}$$

This equation is equivalent to

$$N2\arctan\left(\cot\frac{\Theta}{2}\tanh\frac{\eta_\alpha}{2}\right) = 2\pi J_\alpha + \sum_{\beta=1}^{r} 2\arctan\left(\cot\Theta\tanh\frac{\eta_\alpha-\eta_\beta}{2}\right) \tag{2.7b}$$

where the J_α-s are integers if $N-r$ is odd and half odd-

-integers if $N-r$ is even. In the following we will use (2.7b).

The energy of the state expressed in terms of these new variables is

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

The momentum is

$$p = \sum_{\alpha=1}^{r} k_\alpha = \frac{2\pi}{N}\sum_{\alpha=1}^{r} \lambda_\alpha = -\frac{2\pi}{N}\sum_{\alpha=1}^{r} J_\alpha + r\pi \tag{2.9}$$

2.2 The ground state

The ground state belongs to the $S^z = 0$ subspace if N is even and to the $S^z = 1/2$ if N is odd. For the sake of simplicity we will always suppose that N is even. Then in order to describe the ground state one has to choose the $J_\alpha(\lambda_\alpha)$ set (des Cloizeaux and Gaudin (1966)) as

$$\begin{aligned} J_\alpha &= -\frac{1}{2}\left(\frac{N}{2} + 1 - 2\alpha\right) \qquad \alpha = 1, 2, \ldots, N/2 \\ \lambda_\alpha &= 2\alpha - 1 \end{aligned} \tag{2.10}$$

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

With these quantum numbers all k_α-s (η_α-s) will be real. In the large N limit the equation obtained from (2.7) for $\sigma(\eta)$, the density of η_α -s ($N\sigma(\eta)d\eta$ is the number of η_α -s in the interval $(\eta, \eta+d\eta)$) yields

$$\sigma_0(\eta) = \frac{1}{4\Theta} \cdot \frac{1}{\cosh(\eta\pi/4\Theta)} \tag{2.11}$$

The ground state energy is

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

2.3 Extension to complex η -s

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 for which all k_α-s are real and

$$\Theta < k_\alpha < 2\pi - \Theta \tag{2.13}$$

for all k_α-s. An argument supporting this is that in the planar limit $(\rho=0 \ , \ \Theta=\pi/2)$ the only $S^z=0$ state with all k_α falling into the region $(\pi/2 \ ; 3\pi/2)$ 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 (2.6a) defines real η -s for k -s satisfying (2.13) only, we have to extend (2.6) to complex variables too. In doing this, we will use the definitions

$$2\arctan(\cot\Theta \tanh(\varphi + i\chi)) =$$

$$\left\{2\arctan(\cot\Theta\tanh(\varphi+i\chi))\right\}_{cont} + \left\{2\arctan(\cot\Theta\tanh(\varphi+i\chi))\right\}_{discont} \tag{2.14a}$$

$$\left\{2\arctan(\cot\Theta\tanh(\varphi+i\chi))\right\}_{cont} = \frac{1}{2i}\ln\frac{\cosh 2\varphi-\cos 2(\Theta-\chi)}{\cosh 2\varphi-\cos 2(\Theta+\chi)} + \tag{2.14b}$$

$$+\arctan(\cot(\Theta-\chi)\tanh\varphi) + \arctan(\cot(\Theta+\chi)\tanh\varphi)$$

$$\left\{2\arctan(\cot\Theta\tanh(\varphi+i\chi))\right\}_{discont} = \tag{2.14c}$$

$$=\frac{\pi}{2}\,\mathrm{sign}\varphi\left\{\mathrm{sign}(\chi-\Theta)+\mathrm{sign}(\chi-\Theta+\pi)+\mathrm{sign}(-\chi-\Theta)+\mathrm{sign}(-\chi-\Theta+\pi)\right\}$$

Here we understand, that $0<\Theta<\pi$, $-\pi<\chi\leq\pi$ and $|\arctan x|\leq\pi/2$ for real x .

It is not hard to see, that complex k -s correspond to complex η -s with $|\mathrm{Im}\,\eta|<\pi$, while real k -s not satisfying (2.13) are described by complex η-s with $\mathrm{Im}\,\eta=\pi$. As in any $S^z=0$ excited state some of the k -s must be complex or real but not satisfying (2.13), in order to find $S^z=0$ excitations we will look for such solutions of Eq. (2.7b) in which some of the η -s are complex with $-\pi<\mathrm{Im}\,\eta\leq\pi$. In doing this our strategy will be the following: we write Eqs. (2.7b) both for the real and complex η -s. The equations for the real η -s will be solved for the density of these variables. By means of this density, the real η -s can be eliminated from the equations for the complex η -s leading to the set of equations:

$$\sum_{h=1}^{H} 2\arctan\left(\cot\left(\frac{\Theta}{2}\cdot\frac{\pi}{\pi-\Theta}\right)\tanh\left(\frac{\psi_n-\eta_h}{2}\,\frac{\pi}{\pi-\Theta}\right)\right) = 2\pi J_n' + \tag{2.15}$$

$$+\sum_{m=1}^{H/2} 2\arctan\left(\cot\left(\Theta\cdot\frac{\pi}{\pi-\Theta}\right)\tanh\left(\frac{\psi_n-\psi_m}{2}\cdot\frac{\pi}{\pi-\Theta}\right)\right) \qquad ((3.22))$$

Here the set of auxiliary variables ψ_n represents the complex η -s (see (3.19) and (3.20)) and the η_h variables are the positions of the holes in the real η distribution. The equations determining the η_h variables will be found to be of the form:

$$N\cdot 2\cdot\arctan\left(\tanh\frac{\eta_h\pi}{4\Theta}\right) = 2\pi J_h'' - \sum_{h'=1}^{H} \phi\left((\eta_h-\eta_{h'})\frac{\pi}{\pi-\Theta}\right) + \tag{2.16}$$

$$+\sum_{n=1}^{H/2} 2\arctan\left(\cot\left(\frac{\Theta}{2}\cdot\frac{\pi}{\pi-\Theta}\right)\cdot\tanh\left(\frac{\eta_h-\psi_n}{2}\cdot\frac{\pi}{\pi-\Theta}\right)\right) \qquad ((3.25))$$

where ϕ is a monotonically increasing function of its argument, varying between $\pm(\pi-2\Theta)/(2\cdot(\pi-\Theta))$ (see (3.26)).

After deducing the above set of equations (Section 3.) we will solve them in Section 4. for the case when the number of η_h-s is two. Two classes of solutions will be found, one corresponding to states with a complex k pair, the other corresponding to states with one real k outside of the region $(\Theta;2\pi-\Theta)$. The former states are singlets, while the later ones are triplets in the isotropic limit.

3. EQUATIONS FOR THE STATES WITH SEVERAL COMPLEX η-s

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

3.1 Density of the real η-s

Eq. (2.7b) for the real η -s can be written in the form

$$N.2\arctan\left(\cot\frac{\Theta}{2}\tanh\frac{\eta_\alpha}{2}\right) = 2\pi J'_\alpha + \sum_\beta 2\arctan\left(\cot\Theta\tanh\frac{\eta_\alpha-\eta_\beta}{2}\right) + \tag{3.1}$$

$$+ \sum_n\left\{2\arctan\left(\cot\Theta\tanh\frac{\eta_\alpha-\eta_n}{2}\right)\right\}_{cont}$$

where we introduced

$$J'_\alpha = J_\alpha + \frac{1}{2\pi}\sum_n\left\{2\arctan\left(\cot\Theta\tanh\frac{\eta_\alpha-\eta_n}{2}\right)\right\}_{discont} \tag{3.2}$$

all J'_α -s are integers if $N/2 - n_3$ is odd and they are half odd-integers otherwise. If in Eq. (3.1) we put all terms onto the l.h.s. except for $2\pi J'_\alpha$, we find that its value is between

+ and $-\pi(N/2+2n_2+n_3)$. Taking into account also the restriction on the parities of the $2\mathcal{I}'_\alpha$ numbers we find that the largest and smallest possible values for the $\mathcal{I}'_\alpha$-s are + and $-(1/2)(N/2+2n_2+n_3-1)$ respectively. Thus, to have an $S^2=0$ state $(r=N/2)$, for the $\mathcal{I}'_\alpha$ set we have to choose $N/2-2n_1-2n_2-n_3$ different numbers from the set:

$$-\frac{1}{2}\left(\frac{N}{2}+2n_2+n_3-1\right), -\frac{1}{2}\left(\frac{N}{2}+2n_2+n_3-3\right), \ldots, \frac{1}{2}\left(\frac{N}{2}+2n_2+n_3-1\right) \qquad (3.3)$$

It can be shown (see Appendix A) that for such a choice of the $\mathcal{I}'_\alpha$ -s Eq. (3.1) has a solution. Equation (3.1) defines η-s (later on denoted by η_h-s) also for the $2n_1+4n_2+2n_3=H$ $\mathcal{I}'_h$-s (the numbers left out of the set (3.3)):

$$N.2\arctan\left(\cot\frac{\Theta}{2}\tanh\frac{\eta_h}{2}\right) = 2\pi\mathcal{I}'_h + \sum_\beta 2\arctan\left(\cot\Theta\tanh\frac{\eta_h-\eta_\beta}{2}\right)$$
$$+\sum_n\left\{2\arctan\left(\cot\Theta\tanh\frac{\eta_h-\eta_n}{2}\right)\right\}_{cont} \qquad (3.4)$$

The density of the η_α-s satisfying (3.1) with the above choice of the $\mathcal{I}'_\alpha$ -s must satisfy the equation

$$\frac{\sin\Theta}{\cosh\eta-\cos\Theta} = 2\pi\left(\sigma(\eta)+\frac{1}{N}\sum_h\delta(\eta-\eta_h)\right)+\int_{-\infty}^{\infty}\frac{\sin 2\Theta}{\cosh(\eta-\eta')-\cos 2\Theta}\,\sigma(\eta')\,d\eta'$$
$$+\frac{1}{N}\sum_n\frac{\sin 2\Theta}{\cosh(\eta-\eta_n)-\cos 2\Theta} \qquad (3.5)$$

which, when solved by Fourier transformation yields

$$\sigma(\eta) = \sigma_0(\eta) + \frac{1}{N}\sigma_1(\eta) + \frac{1}{N}\sigma_2(\eta) \qquad (3.6)$$

where $\sigma_0(\eta)$ is the ground state density given by (2.11); and $\sigma_1(\eta)$ and $\sigma_2(\eta)$ are given as

$$\sigma_1(\eta) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left\{-\frac{\sinh\omega\pi}{2\sinh\omega(\pi-\Theta)\cdot\cosh\omega\Theta}\right\}\sum_h e^{i\omega(\eta-\eta_h)}\,d\omega \tag{3.7}$$

$$\sigma_2(\eta) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\sum_n\left\{-\frac{f(2\Theta;-\chi_n)}{2\sinh\omega(\pi-\Theta)\cosh\omega\Theta}\right\}e^{i\omega(\eta-\varphi_n)}\,d\omega \tag{3.8}$$

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

$$f(\Theta;\chi) = \sinh\omega\pi\cdot\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i\omega\varphi}\frac{\sin\Theta}{\cosh(\varphi+i\chi)-\cos\Theta}\,d\varphi \tag{3.9}$$

Its form for $\Theta<\pi$ is

$$f(\Theta;\chi) = \begin{cases} e^{-\omega(\chi-2\pi)}\cdot\sinh\omega(\pi-\Theta) & 2\pi-\Theta<\chi\le 2\pi \\ -e^{-\omega(\chi-\pi)}\cdot\sinh\omega\Theta & \Theta<\chi<2\pi-\Theta \\ e^{-\omega\chi}\cdot\sinh\omega(\pi-\Theta) & -\Theta<\chi<\Theta \\ -e^{-\omega(\chi+\pi)}\cdot\sinh\omega\Theta & -(2\pi-\Theta)<\chi<-\Theta \\ e^{-\omega(\chi+2\pi)}\cdot\sinh\omega(\pi-\Theta) & -2\pi\le\chi<-(2\pi-\Theta) \end{cases} \tag{3.10a}$$

and for $\pi<\Theta<2\pi$ it is

$$f(\Theta;\chi) = \begin{cases} e^{-\omega(\chi-2\pi)}\cdot\sinh\omega(\pi-\Theta) & \Theta<\chi\le 2\pi \\ e^{-\omega(\chi-\pi)}\cdot\sinh\omega(2\pi-\Theta) & 2\pi-\Theta<\chi<\Theta \\ e^{-\omega\chi}\cdot\sinh\omega(\pi-\Theta) & -(2\pi-\Theta)<\chi<2\pi-\Theta \\ e^{-\omega(\chi+\pi)}\cdot\sinh\omega(2\pi-\Theta) & -\Theta<\chi<-(2\pi-\Theta) \\ e^{-\omega(\chi+2\pi)}\cdot\sinh\omega(\pi-\Theta) & -2\pi\le\chi<-\Theta \end{cases} \tag{3.10b}$$

(We give the form of $f(\Theta;\chi)$ in the full $0<\Theta<2\pi$, $|\chi|<2\pi$ region as in later calculations this will be needed.)

3.2 Equations for the complex η-s

Eq. (2.7b) for a complex η takes the form

$$N.2.\arctan\left(\cot\frac{\Theta}{2}\tanh\frac{\eta_n}{2}\right) = 2\pi J_n + \sum_\beta 2\arctan\left(\cot\Theta\tanh\frac{\eta_n-\eta_\beta}{2}\right) + \sum_m 2\arctan\left(\cot\Theta\tanh\frac{\eta_n-\eta_m}{2}\right) \qquad (3.11)$$

If we replace the continuous part of the second term on the r.h.s. by

$$N.\int_{-\infty}^{\infty}\left\{2\arctan\left(\cot\Theta\tanh\frac{\eta_n-\eta'}{2}\right)\right\}_{cont}\cdot\sigma(\eta')\,d\eta' \qquad (3.12)$$

after some algebra we get

$$\left.\begin{array}{ll} N.2\arctan\left(\tanh\frac{\eta_n\pi}{4\Theta}\right) & (\text{if } |\chi_n|<2\Theta) \\ N.2.\operatorname{sign}\varphi_n & (\text{if } |\chi_n|>2\Theta) \end{array}\right\} = 2\pi J_n + \sum_\beta\left\{2\arctan\left(\cot\Theta\tanh\frac{\eta_n-\eta_\beta}{2}\right)\right\}_{discont} + \int_{-\infty}^{\infty}\left\{2\arctan\left(\cot\Theta\tanh\frac{\eta_n-\eta'}{2}\right)\right\}_{cont}\times(\sigma_1(\eta')+\sigma_2(\eta'))\,d\eta' + \sum_m 2\arctan\left(\cot\Theta\tanh\frac{\eta_n-\eta_m}{2}\right) \qquad (3.13)$$

What is interesting for us is the imaginary part of the l.h.s.

of the above equation: It has a value proportional to N if $|\chi_n| < 2\Theta$ and it is zero if $|\chi_n| > 2\Theta$. In the first case Eq. (3.13) can be satisfied only if at the same time the r.h.s. has an imaginary part of the order of N, that is, for the η_n with $|\chi_n| < 2\Theta$ there is another $\eta_{n'}$ for which

$$2\arctan\left(\cot\Theta \tanh \frac{(\varphi_n + i\chi_n) - (\varphi_{n'} + i\chi_{n'})}{2}\right) \tag{3.14}$$

is of the order of N, i.e. (see Eq. (2.14b))

$$(\varphi_n - \varphi_{n'}) + i(\chi_n - \chi_{n'}) = \pm i2\Theta + 2\delta \tag{3.15}$$

with δ being exponentially small in N. As the term (3.14) appears also on the r.h.s. of Eq. (3.13) for $\eta_{n'}$ (with a minus sign) it is clear that also $|\chi_{n'}|$ must be less than 2Θ. Thus we conclude that the set of complex η_n -s with $|\chi_n| < 2\Theta$ must consist of pairs satisfying Eq. (3.15), that is pairs of the form

$$\begin{aligned} \eta_n^+ &= \varphi_n + i(\mu_n + \Theta) + \delta_n \\ & \qquad\qquad\qquad\qquad |\mu_n| < \Theta \\ \eta_n^- &= \varphi_n + i(\mu_n - \Theta) - \delta_n \end{aligned} \tag{3.16}$$

We note, that since all η_n with $|\chi_n| < \pi$ must appear in the complex η set together with its complex conjugate (3.16) implies also, that the set of η_n -s with $|\chi_n| < 2\Theta$ must consist of i/ complex conjugate pairs of the form

$$\eta_n^+ = \varphi_n + i(\Theta+\delta) \quad ; \quad \eta_n^- = \varphi_n - i(\Theta+\delta) \qquad (\mu_n = 0) \tag{3.17}$$

ii/ and quartets of the form

$$\begin{aligned} \eta_n^+ &= \varphi_n + i(\mu_n+\Theta) + \delta_n \quad ; \quad \eta_n^- = \varphi_n + i(\mu_n-\Theta) - \delta_n \\ \eta_{n'}^+ &= \varphi_n + i(-\mu_n+\Theta) - \delta_n^* \quad ; \quad \eta_{n'}^- = \varphi_n + i(-\mu_n-\Theta) + \delta_n^* \end{aligned} \tag{3.18}$$

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:

α / one complex η pair, η_n^+ and η_n^- of the form of (3.16) is represented by a single ψ_n

$$\psi_n = \varphi_n + i\mu_n \qquad |\mu_n| < \Theta \tag{3.19}$$

β / a complex η_n with $|\chi_n| > 2\Theta$ is represented by a ψ_n of the form

$$\psi_n = \varphi_n + i\mu_n \qquad \Theta < |\mu_n| \le \pi - \Theta \tag{3.20a}$$

with

$$\mu_n = \begin{cases} x_n - \Theta & \text{if} \quad \pi \ge x_n > 2\Theta \\ x_n + \Theta & \text{if} \quad -2\Theta > x_n > -\pi \end{cases} \tag{3.20b}$$

The set of ψ_n -s consists of real numbers, complex conjugate pairs and complex numbers of the form $\varphi + i(\pi-\Theta)$. The number of all ψ_h -s is $n_1+2n_2+n_3 = H/2$, that is half of the number of "holes" in the real η distribution.

Using the definition of ψ_n -s, $\sigma_2(\eta)$, the part of $\sigma(\eta)$ that corresponds to the complex η -s can be written in a simpler form:

$$\sigma_2(\eta) = -\frac{\pi}{\pi-\Theta} \cdot \sum_n \frac{\sin(\Theta\pi/(\pi-\Theta))}{\cosh((\eta-\psi_n)\cdot\pi/(\pi-\Theta)) - \cos(\Theta\pi/(\pi-\Theta))} \tag{3.21}$$

The equation for a ψ_n with $|\mu_n| < \Theta$ can be obtained by summing up Eq. (3.13) 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-s can be neglected (see: Appendix B). The equations for the ψ_n -s with $|\mu_n| > \Theta$ are obtained simply by rearranging the terms in Eq. (3.13) for the corresponding η_n -s, and neglecting the exponentially small δ -s. As a result we get for all ψ_n -s:

$$\sum_{h=1}^{H} 2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\psi_n'-\eta_h'}{2}\right) = 2\pi J_n' + \sum_{m=1}^{H/2} 2\arctan\left(\cot\Theta'\tanh\frac{\psi_n'-\psi_m'}{2}\right) \qquad \begin{matrix}(3.22)\\((2.15))\end{matrix}$$

Here we used the notations

$$\Theta' = \frac{\pi}{\pi-\Theta}\cdot\Theta \;\; ; \;\; \eta_h' = \frac{\pi}{\pi-\Theta}\cdot\eta_h \;\; ; \;\; \psi_n' = \frac{\pi}{\pi-\Theta}\cdot\psi_n = \varphi_n' + i\mu_n' \tag{3.23}$$

The J_n' parameters were obtained by collecting the terms of the form $n\cdot\pi$; their connections with the original $\mathcal{I}_n$ -s are

$$\mathcal{I}_n' = \mathcal{I}_n^+ + \mathcal{I}_n^- - \frac{N}{2}\,\mathrm{sign}\,\varphi_n + \frac{1}{2}\sum_{m\neq n} \mathrm{sign}(\varphi_n - \varphi_m) \tag{3.24a}$$

for the ψ_n' -s with $|\mu_n'| < \Theta'$ and

$$\mathcal{I}_n' = \mathcal{I}_n - \frac{N}{2}\,\mathrm{sign}\,\varphi_n + \sum_\beta \frac{1}{2}\,\mathrm{sign}(\varphi_n - \eta_\beta) + \frac{1}{2}\sum_h \mathrm{sign}(\varphi_n - \eta_h) + \frac{1}{2}\sum_{|\mu_m|<\Theta} \mathrm{sign}(\varphi_n - \varphi_m) \tag{3.24b}$$

for the ψ_n -s with $|\mu_n'| > \Theta'$. The parity of the numbers $2\mathcal{I}_n'$ is the same as the parity of $H/2 - 1$.

3.3 Equations for the variables η_h

The equations for the η_h-s can be obtained from Eq. (3.4) by replacing the sum over the η_β -s on the r.h.s. by an integral over the η -s with density $N\,\sigma(\eta)$. This way one gets

$$N.2.\arctan\left(\tanh\frac{\eta_h'\pi}{4\Theta'}\right) = 2\pi\,\mathcal{I}_h'' - \sum_{h'}\phi(\eta_h' - \eta_{h'}') + \sum_n 2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\eta_h' - \psi_n'}{2}\right) \tag{3.25}$$

Here we used the notations

$$\phi(x) = \int_{-\infty}^{\infty}\frac{d\omega}{i\omega}\cdot\frac{\sinh\omega(\pi-\Theta')}{2\sinh\omega\pi\,\cosh\omega\Theta'}\cdot e^{i\omega x} \tag{3.26}$$

and

$$\mathfrak{I}_h'' = \mathfrak{I}_h' - \frac{1}{2\pi}\sum_n \left\{2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\eta_h' - \psi_n'}{2}\right)\right\}_{discont} \qquad (3.27)$$

The $\mathfrak{I}_h''$ 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 (3.22) and (3.25)

By solving the system (3.22) (3.25) one can construct the solution of the original Eq. (2.7): if the ψ_n-s are given, according to Eqs. (3.16) (3.19) and (3.20) the complex η-s can be calculated (up to exponentially small terms) and knowing also the η_h-s through Eqs. (3.6) (3.7) and (3.21) the density of the η_κ-s can be determined too.

The system (3.22) and (3.25) can be used to calculate the excited states of an isotop $(\rho=1)$ Heisenberg chain too. For this we have to take the $\Theta \to 0$ limit. In this limit all η variables (except those complex η-s for which $\chi = \pi$) desappear proportionally to Θ while the η/Θ $(= \cot(k/2))$ ratios remain finite. From the complex η-s with $\chi = \pi$ only the "discount" parts of the $\arctan$ functions remain. It is not hard to check that this procedure leads to the same equations as the procedure described in Subsections 3.1-3.3 applied directly on the secular equations of the isotrop Heisenberg chain.

In a strict sense Eqs. (3.22) and (3.25) are equivalent to the original Eq. (2.7) only if the number of excitations (H) is small compared to N. The reason for this is that we used (implicitely) the smallness of H at two points. One point is, that the solution of Eq. (3.5) describes the density of the η_α -s satisfying (3.1) only if $\sigma(\eta)+(1/N)\Sigma_h\delta(\eta-\eta_h)$ is poistive for all η, that is

$$\sigma_0(\eta)+\frac{1}{N}\int_{-\infty}^{\infty}\frac{\sinh\omega(\pi-2\Theta)}{2\sinh\omega(\pi-\Theta)\cosh\omega\Theta}\cdot\sum_h e^{i\omega(\eta-\eta_h)}d\omega+\frac{1}{N}\sigma_2(\eta)>0 \qquad (3.28)$$

One can be sure of the validity of (3.28) only if the number of excitations is small, otherwise the $(1/N)\cdot\sigma_2(\eta)$ term (which can be negative) may make the whole expression negative for some η -s. The other point where we used the smallness of H was when we argued that in order to satisfy Eq. (3.13) the set of complex η -s with $|x|<2\Theta$ must consist of pairs of the form (3.16). If the number of excitations (the number of terms on the r.h.s. of (3.13)) is comparable to N, the imaginary part of the r.h.s. of (3.13) can be of the order of N even if no term in itself is of the order of N, thus we cannot argue that we must have a term (3.14) with an argument satisfying (3.15). Thus to generalise our results for the case of large (macroscopic) H, one can do the following: after solving Eqs. (3.22) (3.25) for the η_h -s and ψ_n -s one should check wether (3.28) is satisfied. If it is, than one should calculate the δ -s (see Appendix B). If they are of the order of e^{-N}, then the solution of (3.22) (3.25) indeed corresponds to a solution of (2.7), otherwise it does not.

The original Eq. (2.7) is expected to have solutions in which some of the complex η-s can be arranged into series of the types $\eta_{\pm m} \cong \varphi \pm i(2m+1)\Theta$ and $\eta_{\pm m} \cong \varphi \pm i\,2m\Theta$, $(m=0,1,2,\dots,n)$. These sorts of "strings" correspond to series of ψ'-s of the form $\psi'_{\pm m} \cong \varphi' \pm i2m\Theta'$ and $\psi'_{\pm m} \cong \varphi' \pm i(2m-1)\Theta'$. It is not hard to see, that such string solutions of Eq. (3.22) can exist only if the number of η_h-s is sufficiently large. If H is small, there is no reason for having terms with large imaginary parts on the r.h.s. of (3.22). In this case, however, we may have ψ'_n-s with $|\mu'_n| < \Theta'$ which correspond to quartets of the form $\varphi_n \pm i(\mu_n \pm \Theta)$.

3.5 Energy and momentum of the states with complex η-s.

The energy is calculated according to the formula (2.8) which in our case takes the form

$$E = -\sum_{\alpha} \frac{\sin^2\Theta}{\cosh\eta_\alpha - \cos\Theta} - \sum_{|\mu_n|<\Theta}\left(\frac{\sin^2\Theta}{\cosh\eta_n^+ - \cos\Theta} + \frac{\sin^2\Theta}{\cosh\eta_n^- - \cos\Theta}\right) - \sum_{|\mu_n|>\Theta} \frac{\sin^2\Theta}{\cosh\eta_n - \cos\Theta} \tag{3.29}$$

If the first term is evaluated by means of $\sigma(\eta)$; (3.29) yields

$$E = E_0 + \frac{\pi}{2}\cdot\frac{\sin\Theta}{\Theta}\cdot\sum_h \frac{1}{\cosh(\eta_h\pi/2\Theta)} \tag{3.30}$$

with E_0 given by (2.12).

The momentum, using (2.9), (3.2), (3.3), (3.23), (3.24), (3.25) and (3.27) is

$$p = \sum_h -p_h + \sum_n \pi(1 - \operatorname{sign}\varphi_n) + \frac{N}{2}\pi \tag{3.31}$$

with

$$0 < p_h = \frac{\pi}{2} - 2\arctan\left(\tanh\frac{\eta_h \pi}{4\Theta}\right) < \pi \tag{3.32}$$

Comparing (3.30) and (3.32) and finds that

$$E - E_0 = \sum_h \frac{\pi}{2} \cdot \frac{\sin\Theta}{\Theta} \cdot \sin p_h \quad ; \quad p - p_0 = \sum_h -p_h \pmod{2\pi} \tag{3.33}$$

The form (3.33) of the energy and momentum suggests that the states with complex η -s can be interpreted as states with some sort of quasi-particles present. Interestingly, the number of these quasi-particles is not the number of complex η -s, but the number of holes in the real η distribution, i.e. H . These quasi-particles are, however, interacting ones, this is expressed by the fact that the momenta are not free parameters, they are coupled to the quantum numbers ($\mathfrak{Z}_h''$ and $\mathfrak{Z}_n'$) by the system (3.22) (3.25).

4. THE SIMPLEST EXCITED STATES: THE STATES WITH TWO HOLES IN THE REAL η DISTRIBUTION

4.1 States with one real ψ'

For $H=2$ the numbers of ψ'-s is one, this means that ψ' must be either real or of the form $\varphi'+i\pi$. Now we treat the first case. For a real $\psi'=\varphi'$ Eq. (3.22) takes the form

$$2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\varphi'-\eta'_{h_1}}{2}\right)+2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\varphi'-\eta'_{h_2}}{2}\right)=2\pi J' \qquad (4.1)$$

This equation has a solution only if $J'=0$, then

$$\varphi'=(\eta'_{h_1}+\eta'_{h_2})/2 \quad ; \quad \varphi=(\eta_{h_1}+\eta_{h_2})/2 \qquad (4.2)$$

which corresponds to a complex η and k pair

$$\eta^{\pm}=(\eta_{h_1}+\eta_{h_2})/2 \pm i\Theta \qquad (4.3)$$

$$k^{\pm}=\left(\frac{\pi}{2}(2-\operatorname{sign}\varphi)-\arctan\left(\cot\Theta\tanh\frac{\varphi}{2}\right)\right)\pm\frac{i}{2}\ln\frac{\cosh\varphi-1}{\cosh\varphi-\cos2\Theta} \qquad (4.4)$$

with φ' given by (4.2) Eq. (3.25) can be solved numerically for η_{h_1} and η_{h_2} if J''_{h_1} and J''_{h_2} are two different numbers between $\pm(1/2)(N/2-1)$. The number of possibilities is $N(N-1)/2$.

The energy-momentum dispersion, according to (3.33) is

$$E - E_0 = \frac{\pi}{2}\cdot\frac{\sin\Theta}{\Theta}\cdot \sin p_{h_1} + \frac{\pi}{2}\cdot\frac{\sin\Theta}{\Theta}\cdot \sin p_{h_2} \tag{4.5}$$

that is, the continuum of this excitations in the $(\epsilon; p)$ plane (in the reduced Brillouin-zone) is bounded by the curves

$$\pi\cdot\frac{\sin\Theta}{\Theta}\cdot\sin(|p|/2) \quad ; \quad \frac{\pi}{2}\cdot\frac{\sin\Theta}{\Theta}\cdot\sin(|p|) \tag{4.6}$$

The states corresponding to the above solution of Eq. (3.22) in the $\rho \to 1$ $(\Theta \to 0)$ isotropic limit go over into singlet states with one complex k pair. (In this limit the φ/Θ ratio remains finite, thus both the real and imaginary parts of the $k^{\pm}$ remain finite.) Earlier Ovchinnikov (1969) presented a calculation for the singlet excitations of the isotropic antiferomagnetic Heisenberg chain. He claimed that these excitations have the dispersion $\epsilon(p) = \pi\cdot|\sin(p/2)|$ with $|p| < \pi/2$. Fazekas and Sütõ (1976) diagonalized $\hat{H}$ of (1.1) with $\rho = 1$ in the singlet subspace numerically for finite chains and extrapolated their results for $N \to \infty$. They found that the lower edge of the singlet continuum is described by the dispersion $\epsilon(p) = (\pi/2)|\sin p|$. Our analitic result coincides with that of Fazekas and Sütõ.

It is also interesting to examine the above states in the $\rho \to 0$ $(\Theta \to \pi/2)$ planar limit. At first sight it is surprising that the imaginary parts of the complex k-s do not vanish, which would indicate that we have some sort of bound states, even if the interaction part of (1.1) vanishes. A closer look, however, shows that there are no bound states in this limit. The easiest way to describe these states is in the equivalent fermion picture ($c_n^+ = S_n^- \cdot \exp\{i\pi \sum_{j=1}^{n-1} (S_j^z - 1/2)\}$; $|F\rangle = |vacuum\rangle$). It is not hard to verify, that the limiting form of the states with one complex k pair of (4.4) is

$$\left\{ \frac{\sin p_1}{\coth\varphi - \cos p_1} \cdot c^+_{\frac{\pi}{2}-p_1} \cdot c_{\frac{\pi}{2}+p_2} - \frac{\sin p_2}{\coth\varphi - \cos p_2} \cdot c^+_{\frac{\pi}{2}-p_2} \cdot c_{\frac{\pi}{2}+p_1} \right\} |0\rangle \qquad (4.7)$$

where p_1 and p_2 stand for p_{h_1} and p_{h_2} of (3.33) respectively, c_k is the Fourier transform of c_n , and $|0\rangle$ is the ground state i.e. the state with all modes between $\pi/2$ and $3\pi/2$ filled in.

4.2 The states with one complex ψ' of the form $\varphi' + i\pi$

The second class of the solutions of Eq. (3.22) is the one with a complex $\psi' = \varphi' + i\pi$. In this case Eq. (3.22) is

$$2\arctan\left(\cot\frac{\Theta'}{2}\coth\frac{\varphi' - \eta'_{h_1}}{2}\right) + 2\arctan\left(\cot\frac{\Theta'}{2}\coth\frac{\varphi' - \eta'_{h_2}}{2}\right) = 2\pi \mathfrak{J}' \qquad (4.8)$$

which again has a solution only if $\mathfrak{J}' = 0$:

$$\varphi' = (\eta'_{k_1} + \eta'_{k_2})/2 \quad ; \quad \varphi = (\eta_{k_1} + \eta_{k_2})/2 \tag{4.9}$$

Now the complex η is

$$\eta = \varphi' \cdot \frac{\pi - \Theta}{\pi} + \Theta = (\eta_{k_1} + \eta_{k_2})/2 + i\pi \tag{4.10}$$

corresponding to a real k

$$k = \pi(1 - \mathrm{sign}\,\varphi) + 2\arctan\left(\tan\frac{\Theta}{2}\tanh\frac{\varphi}{2}\right) \tag{4.11}$$

which falls into one of the regions $(0;\Theta)$ and $(2\pi-\Theta;2\pi)$. With φ' given Eq. (3.25) can be solved if $\mathcal{I}''_{k_1}$ and $\mathcal{I}''_{k_2}$ are two (different or equal) numbers between $\pm(1/2)(N/2-1)$. The number of different solutions is $N(N+1)/2$. The energies of these states are given also by (4.5).

We note that the above described class of states involve (treated in a more accurate way) the $S^z = 0$ excitations found by des Cloizeaux and Gaudin (1966). Their excitation can be obtained by taking p_{k_1} or p_{k_2} equal to zero (or π).

The states with one complex $\eta = \varphi + i\pi$ go over into the $S^z = 0$ triplet excitations (k of (4.11) becomes equal to 0 or 2π) described by Yamada (1969) as $\rho \to 1$.

It is not hard to verify that the states discussed in this subsection in the planar limit go over into the states (expressed in the equivalent fermion representation)

$$\left\{ \frac{\sin p_1}{\tanh\varphi - \cos p_1} \cdot c^{+}_{\frac{\pi}{2}-p_1} \cdot c_{\frac{\pi}{2}+p_2} - \frac{\sin p_2}{\tanh\varphi - \cos p_2} \cdot c^{+}_{\frac{\pi}{2}-p_2} \cdot c_{\frac{\pi}{2}+p_1} \right\} |0\rangle \tag{4.12}$$

if $\mathcal{J}''_{h_1}$ and $\mathcal{J}''_{h_2}$ are different, and, into the states

$$c^{+}_{\frac{\pi}{2}-p}\, c_{\frac{\pi}{2}+p}\, |0\rangle \tag{4.13}$$

if $\mathcal{J}''_{h_1} = \mathcal{J}''_{h_2}$ $\left(\mathcal{J}'_{h_1} - \mathcal{J}'_{h_2} = 1 \right)$. The states of (4.12) and (4.7) with the same p_1, p_2 pair are, as they should be, orthogonal.

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 $0 \leq \varrho \leq 1$. Our study has been based on the secular equations for the problem (Eq. (2.7)).

It has been argued, that to describe the $S^z = 0$ excitations complex η parameters should be introduced. From the original Eq. (2.7) a simpler system (Eqs. (3.22) (3.25)) has been deduced. This system contains only the parameters of the excitations: the ψ -set which represents the complex η -s and the positions of the holes in the real η distribution. The energy-momentum dispersion is also determined. Its form is $p = \sum_h -p_h$, $\epsilon = \sum_h (\pi/2)(\sin\Theta/\Theta) \cdot \sin p_h$, where the p_h momenta are determined by the holes in the real η distribution (Eq. (3.32)). It is remarkable, that the complex η -s do not appear explicitely in the energy expression. The form of the energy and the momentum suggests, that the states in question can be regarded as states with quasi-particles of momenta p_h present. This quasi particles are interacting ones, since their momenta are not free parameters, they are determined by the system of equations (3.22) and (3.25).

It has been a general opinion, that the complex η -s obtainable as solutions of the secular equations (2.7) can be arranged into strings of the form $\eta_m = \varphi \pm i2m\Theta$, (the m-s being integers or half odd-integers). A simple argument based on the form of Eq. (3.22) shows, however, that string-solutions (except the $\varphi \pm i\Theta$ ones) can exist only if the number of holes in the real η distribution is sufficiently large. If the number of holes is small, instead of the longer strings complex η configurations of the type $\varphi \pm i(\mu \pm \Theta)$ $(|\mu| < \Theta)$ can appear.

Solutions for the system (3.22) (3.25) are obtained in the simplest case, when the number of holes is two. In this case two classes of solutions exist. In one of them the wavenumber set consists of $N/2-2$ real k-s falling into the region $(\Theta; 2\pi-\Theta)$ and a pair of complex wavenumbers. These states in the $\varrho=1$ isotropic limit coincide with the simplest singlet excitations of the chain. They are characterized by two parameters, and their continuum in the $(\varepsilon; p)$ plane is bounded by the curves $(\pi/2).(\sin\Theta/\Theta)\cdot|\sin p|$ and $\pi\cdot(\sin\Theta/\Theta)\cdot|\sin(p/2)|$. In the $\varrho=0$ planar limit the same excitations can be regarded as perticle-hole type ones.

In the other class of excitations of two parameters $N/2-1$ real wavenumbers fall into the region $(\Theta; 2\pi-\Theta)$ while one wavenumber is in one of the regions $(0;\Theta)$, $(2\pi-\Theta; 2\pi)$. In the isotropic limit these states go over into the $S^z=0$ triplet states of the chain, while in the planar limit they also form a set of particle-hole type excitations.

ACKNOWLEDGEMENT

I am very grateful to Drs. A. Sütő and P. Fazekas for the many illuminating discussions and to Dr. J. Sólyom for the critical reading of the manuscript.

APPENDIX A: EXISTENCE OF A SOLUTION FOR Eq. (3.1)

We write Eq. (3.1) in the form

$$N \cdot 2\arctan\left(\cot\frac{\Theta}{2}\tanh\frac{\eta_\alpha}{2}\right) - \sum_{\substack{\pi-2\Theta<x_n<\pi \\ -\pi<x_n<-2\Theta}} \arctan\left(\cot\left(\Theta+\frac{x_n}{2}\right)\tanh\frac{\eta_\alpha-\varphi_n}{2}\right)$$

$$- \sum_{\substack{-\pi<x_n<-\pi+2\Theta \\ 2\Theta<x_n<\pi}} \arctan\left(\cot\left(\Theta-\frac{x_n}{2}\right)\tanh\frac{\eta_\alpha-\varphi_n}{2}\right) = 2\pi \mathcal{J}'_\alpha + \qquad \text{(A.1)}$$

$$+ \sum_\beta 2\arctan\left(\cot\Theta\tanh\frac{\eta_\alpha-\eta_\beta}{2}\right) + \sum_{-2\Theta<x_n<\pi-2\Theta} \arctan\left(\cot\left(\Theta+\frac{x_n}{2}\right)\tanh\frac{\eta_\alpha-\varphi_n}{2}\right)$$

$$+ \sum_{-\pi+2\Theta<x_n<2\Theta} \arctan\left(\cot\left(\Theta-\frac{x_n}{2}\right)\tanh\frac{\eta_\alpha-\varphi_n}{2}\right)$$

At fixed values of the complex η_n-s ($\eta_n = \varphi_n + i x_n$; this summations involve all η_n -s , η_n^+-s and η_n^- -s) both sides of (A.1) are monotonically increasing functions of η_α . This property of (A.1) enables us to regard this equation as a transformation: substituting an η_α set into the r.h.s. we can define a new η'_α set by inverting the function on the l.h.s. and taking it at the value of the r.h.s. This transformation is continuous and if the $\mathcal{J}'_\alpha$ set is such that

$$\mathcal{J}'_{\alpha+1} - \mathcal{J}'_\alpha \geq 1 \quad ; \quad |\mathcal{J}'_\alpha| \leq (1/2)(N/2 + 2n_2 + n_3 - 1) \qquad \text{(A.2)}$$

the transformation has the properties

$$\eta'_{\alpha+1} - \eta'_{\alpha} \geq d \qquad \text{if} \quad \eta_{\alpha+1} - \eta_{\alpha} \geq 0 \tag{A.3}$$

$$\eta_- \leq \eta'_{\alpha} \leq \eta_+ \tag{A.4}$$

where the η_+ and η_- are finite numbers defined by the equations:

$$\text{l.h.s. of (A.1) at } \eta_{\pm} = \pm \Big\{ \pi \cdot (N/2 + 2n_2 + n_3 - 1) + (\pi - \Theta)(N/2 - 2n_1 - 2n_2 - n_3) + \tag{A.5}$$

$$+ \sum_{-2\Theta < \chi_n < \pi - 2\Theta} (\pi/2 - \Theta - \chi_n/2) + \sum_{-\pi + 2\Theta < \chi_n < 2\Theta} (\pi/2 - \Theta + \chi_n/2) \Big\}$$

and d is the reciprocal of the maximum of the derivative of the l.h.s. of (A.1) multiplied by 2π. Thus the transformation maps the

$$\eta_- \leq \eta_{\alpha} \qquad \eta_{\alpha} + d \leq \eta_{\alpha+1} \leq \eta_+ \tag{A.6}$$

closed convex and bounded set onto itself. If so, according to Brouwer's theorem (American Mathematical Society Colloquium Publications, Vol. XXVIII. p. 243.) the transformation must have at least one fixed point i.e. (A.1) and so (3.1) have at least one solution.

APPENDIX B: EQUATIONS FOR THE ψ_n-S AND THE δ_n-S.

Eq. (3.13) for an η_n^+ using the ψ_n variables introduced by (3.19) and (3.20) takes the form

$$N.2\arctan\left(\tanh\frac{\psi_n+i\Theta}{2}\cdot\frac{\pi}{2\Theta}\right) = 2\pi J_n^+ + \int_{-\infty}^{\infty}\left\{2\arctan\left(\cot\Theta\tanh\frac{\psi_n+i\Theta-\eta}{2}\right)\right\}\times$$

$$\times(\sigma_1(\eta)+\sigma_2(\eta))\,d\eta + \sum_{\substack{m\neq n\\ \mu_m<\Theta}} 2\arctan\left(\cot\Theta\tanh\frac{(\psi_n+i\Theta)-(\psi_m-i\Theta)}{2}\right) + \tag{B.1}$$

$$+\sum_{\substack{m\neq n\\ \mu_m>-\Theta}} 2\arctan\left(\cot\Theta\tanh\frac{(\psi_n+i\Theta)-(\psi_m+i\Theta)}{2}\right) + 2\arctan\left(\cot\Theta\tanh(i\Theta+\delta_n)\right)$$

The equation for the corresponding η_n^- is

$$N.2\arctan\left(\tanh\frac{\psi_n-i\Theta}{2}\cdot\frac{\pi}{2\Theta}\right) = 2\pi J_n^- + \int_{-\infty}^{\infty}\left\{2\arctan\left(\cot\Theta\tanh\frac{\psi_n-i\Theta-\eta}{2}\right)\right\}\times$$

$$\times(\sigma_1(\eta)+\sigma_2(\eta))\,d\eta + \sum_{\substack{m\neq n\\ \mu_m<\Theta}} 2\arctan\left(\cot\Theta\tanh\frac{(\psi_n-i\Theta)-(\psi_m-i\Theta)}{2}\right) + \tag{B.2}$$

$$\sum_{\substack{m\neq n\\ \mu_m>-\Theta}} 2\arctan\left(\cot\Theta\tanh\frac{(\psi_n-i\Theta)-(\psi_m+i\Theta)}{2}\right) + 2\arctan\left(\cot\Theta\tanh(-i\Theta-\delta_n)\right)$$

In both of the equations we kept the δ_n -s only if it was necessary to avoid divergence. By summing up (B.1) and (B.2) and using the forms (3.7) and (3.8) for $\sigma_1(\eta)$ and $\sigma_2(\eta)$ together with the identity

$$\left\{2\arctan\left(\cot\Theta\tanh\frac{\varphi+i\chi}{2}\right)\right\}_{cont}=\int_{-\infty}^{\infty}\frac{f(2\Theta;\chi)}{\sinh\omega\pi}\cdot e^{i\omega\varphi}\cdot\frac{d\omega}{i\omega} \tag{B.3}$$

(f given by (3.10)) we get

$$\begin{aligned}
N\cdot\pi\cdot\operatorname{sign}\varphi_n &= 2\pi(\xi_n^+ + \xi_n^-) - \sum_n\int_{-\infty}^{\infty}\frac{f(2\Theta;\mu_n+\Theta)+f(2\Theta;\mu_n-\Theta)}{\sinh\omega\pi}\cdot\frac{\sinh\omega\pi\cdot e^{i\omega(\varphi_n-\eta_n)}}{2\sinh\omega(\pi-\Theta)\cosh\omega\Theta}\cdot\frac{d\omega}{i\omega}+\\
&+\sum_{\substack{m\neq n\\ -\Theta<\mu_m<\Theta}}\int_{-\infty}^{\infty}\left\{\frac{f(2\Theta;\mu_n+\Theta)+f(2\Theta;\mu_n-\Theta)}{\sinh\omega\pi}\cdot\left(-\frac{e^{\omega\mu_m}\sinh\omega(\pi-2\Theta)}{\sinh\omega(\pi-\Theta)}\right)+\right.\\
&\qquad\left.+\frac{f(2\Theta;\mu_n-\mu_m+2\Theta)+2f(2\Theta;\mu_n-\mu_m)+f(2\Theta;\mu_n-\mu_m-2\Theta)}{\sinh\omega\pi}\right\}e^{i\omega(\varphi_n-\varphi_m)}\frac{d\omega}{i\omega}+\\
&+\sum_{\mu_m>\Theta}\int_{-\infty}^{\infty}\left\{\frac{f(2\Theta;\mu_n+\Theta)+f(2\Theta;\mu_n-\Theta)}{\sinh\omega\pi}\cdot\frac{e^{\omega(\mu_m+\Theta-\pi)}\sinh\omega\Theta}{\sinh\omega(\pi-\Theta)}+\right.\\
&\qquad\left.+\frac{f(2\Theta;\mu_n-\mu_m)+f(2\Theta;\mu_n-\mu_m-2\Theta)}{\sinh\omega\pi}\right\}\cdot e^{i\omega(\varphi_n-\varphi_m)}\cdot\frac{d\omega}{i\omega}+\\
&+\sum_{\mu_m<-\Theta}\int_{-\infty}^{\infty}\left\{\frac{f(2\Theta;\mu_n+\Theta)+f(2\Theta;\mu_n-\Theta)}{\sinh\omega\pi}\cdot\frac{e^{\omega(\mu_m-\Theta+\pi)}\sinh\omega\Theta}{\sinh\omega(\pi-\Theta)}+\right.\\
&\qquad\left.+\frac{f(2\Theta;\mu_n-\mu_m+2\Theta)+f(2\Theta;\mu_n-\mu_m)}{\sinh\omega\pi}\right\}\cdot e^{i\omega(\varphi_n-\varphi_m)}\cdot\frac{d\omega}{i\omega}+\phi_n
\end{aligned} \tag{B.4}$$

where we denoted by ϕ_n the discont. parts:

$$\phi_n = \sum_{\substack{m\neq n \\ -\Theta<\mu_m<\Theta \\ -2\pi+4\Theta<\mu_n-\mu_m<2\pi-2\Theta}} \pi\cdot \mathrm{sign}(\varphi_n-\varphi_m) +$$

$$+ \sum_{\substack{\mu_m>\Theta \\ -2\pi+2\Theta<\mu_n-\mu_m<-2\Theta}} \pi\, \mathrm{sign}(\varphi_n-\varphi_m) + \sum_{\substack{\mu_m>\Theta \\ -2\pi+4\Theta<\mu_n-\mu_m<0}} \pi\cdot \mathrm{sign}(\varphi_n-\varphi_m) \tag{B.5}$$

$$+ \sum_{\substack{\mu_m<-\Theta \\ 2\Theta<\mu_n-\mu_m<2\pi-2\Theta}} \pi\cdot \mathrm{sign}(\varphi_n-\varphi_m) + \sum_{\substack{\mu_m<-\Theta \\ 0<\mu_n-\mu_m<2\pi-4\Theta}} \pi\cdot \mathrm{sign}(\varphi_n-\varphi_m)$$

Using the form of the function f ((3.10.a) or (3.10.b)) the integrals can be evaluated leading to Eq. (3.22). The connection between η_n' and the original η_n^+ and η_n^- parameters (3.24.a) can be obtained by comparing the discontinuous part of Eq. (3.22) and ϕ_n of (B.5).

To obtain equations fot the ψ_n-s with $|\mu_n|>\Theta$ we have to treat (3.13) in a similar way: writing up all terms but the discount parts in Fourier-transformed form, collecting the terms containing the same $\psi_n-\psi_m$ differences and evaluating the integrals also leads to Eq. (3.22).

The values of the δ_n-s appearing in the η_n^+-s and η_n^- -s are also interesting for us. Equations for them are obtained by subtracting (B.2) from (B.1). In a similar way as their sum was treated, the difference of (B.1) and (B.2) can be brought to the form

$$N.2\left(\arctan\left(\tanh\frac{\psi_n+i\Theta}{2}\cdot\frac{\pi}{2\Theta}\right)-\arctan\left(\tanh\frac{\psi_n-i\Theta}{2}\frac{\pi}{2\Theta}\right)\right)-2\pi(\mathcal{J}_n^+-\mathcal{J}_n^-)-$$

$$-\sum_h\int_{-\infty}^{\infty}\frac{\sinh\omega(\pi-2\Theta)\sinh\omega\Theta}{\sinh\omega(\pi-\Theta)\cosh\omega\Theta}\,e^{i\omega(\psi_h-\eta_h)}\,\frac{d\omega}{i\omega}\ +$$

$$\tag{B.6}$$

$$+\sum_{m\neq n}\left\{2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\psi_n'-\psi_m'-i\Theta'}{2}\right)-2\arctan\left(\cot\frac{\Theta'}{2}\tanh\frac{\psi_n'-\psi_m'+i\Theta'}{2}\right)\right\}$$

$$-\int_{-\infty}^{\infty}\frac{\sinh^2\omega(\pi-2\Theta)\sinh\omega\Theta}{\sinh\omega\pi\,\sinh\omega(\pi-\Theta)}\cdot\frac{d\omega}{i\omega}=4\arctan\left(\cot\Theta\tanh(i\Theta+\delta_n)\right)$$

If the ψ_n -s (thus the ψ_n' -s) and η_h -s are known, with an appropriate choice of the number $\mathcal{J}_n^+-\mathcal{J}_n^-$ (B.6) can be solved for δ_n . Note, that for the sake of consistency, the parity of the number $\mathcal{J}_n^+-\mathcal{J}_n^-$ must be the same as that of the number $\mathcal{J}_n^++\mathcal{J}_n^-+N/2-1$. It is not hard to see that with this restriction both the choice of $\mathcal{J}_n^+-\mathcal{J}_n^-$ and the solution for δ_n is unique.

The modulus of δ_n is determined by the imaginary part of Eq. (B.6):

$$N.\ln\frac{\cosh\frac{\varphi_n\pi}{2\Theta}-\cos\frac{\mu_n\pi}{2\Theta}}{\cosh\frac{\varphi_n\pi}{2\Theta}+\cos\frac{\mu_n\pi}{2\Theta}}-\sum_h\int_{-\infty}^{\infty}\frac{\sinh\omega(\pi-2\Theta)\sinh\omega\Theta}{\sinh\omega(\pi-\Theta)\cos\omega\Theta}\cdot\frac{\cos\omega(\varphi_n-\eta_h)e^{-\omega\mu_n}}{\omega}\cdot d\omega$$

$$+\frac{1}{2}\ln\frac{(\cosh(\varphi_n'-\varphi_m')-\cos(2\Theta'-\mu_n'+\mu_m'))(\cosh(\varphi_n'-\varphi_m')-\cos(2\Theta+\mu_n'-\mu_m'))}{(\cosh(\varphi_n'-\varphi_m')-\cos(\mu_n'-\mu_m'))^2}-\tag{B.7}$$

$$-\int_{-\infty}^{\infty}\frac{\sinh^2\omega(\pi-2\Theta)\sinh\omega\Theta}{\sinh\omega\pi\,\sinh\omega(\pi-\Theta)}\cdot\frac{d\omega}{\omega}=\ln\frac{|\delta_n|^2}{\sin^2 2\Theta}$$

If we have a small number of excitations $(H \ll N)$ then the l.h.s. is dominated by the first term, which is negative and proportional to N, thus $|\delta_n|$ is indeed of the order of e^{-N}. If, however, the number of excitations is comparable to N, then the other terms can contribute significantly, too. Since the solutions of (3.22) and (3.25) correspond to solutions of the original (2.7) equations only if the δ_n-s are small, for large H (B.7) provides a possibility to check whether or not a solution of (3.22) and (3.25) defines a solution for (2.7).

REFERENCES

H. Bethe, Z. Physik 71, 205 (1931)

J.des Cloizeaux, J.J. Pearson, Phys. Rev. 128, 2131 (1962)

J. des Cloizeaux, M. Gaudin, J. Math. Phys. 7, 1384 (1966)

P. Fazekas, A. Sütő, Solid State Comm. 19, 1045 (1976)

R.B. Griffiths, Phys. Rev. 133, A768 (1964)

L. Hulten, Arkiv. Mat. Astron. Fys. 26A 1. (1938)

R. Orbach, Phys. Rev. 116. 1089 (1959)

A.A. Ovchinnikov, Soviet Phys. JETP 29. 727 (1969)

L.R. Walker, Phys. Rev. 112, 309 (1959)

T. Yamada, Progress of Theor. Phys. 41, 880 (1969)

C.N. Yang, C.P. Yang, Phys. Rev. 150, 321 (1966)

C.N. Yang, C.P. Yang, Phys. Rev. 150, 327 (1966)

C.N. Yang, C.P. Yang, Phys. Rev. 151, 258 (1966)

63.182

Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Kroó Norbert
Szakmai lektor: Sólyom Jenő
Nyelvi lektor: Forgács Gábor
Példányszám: 470 Törzsszám: 81-483
Készült a KFKI sokszorosító üzemében
Felelős vezető: Nagy Károly
Budapest, 1981. szeptember hó