EXCITATION SPECTRUM OF AN ANTIFERROMAGNETIC HEISENBERG CHAIN

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An antiferromagnetic Heisenberg chain of spins with an isotropic interaction is considered. The energy spectrum of the excited bound states is found. For its determination, the Bethe equation[1] is solved in a field of complex momenta. It is shown that the bound state spectrum, to which the singlet excited states of the system also belong, starts from zero (i.e., an energy gap does not exist) and has a termination point. Excitations of a combined type also exist when several excitations of the singlet type coexist in the system along with excitations of the triplet type.[5] The total spin of the system is determined, and a classification of the excited states with respect to the spin and number of bound particles (i.e., with respect to the number of complex momenta) is given.

1. INTRODUCTION

A linear Heisenberg chain of spins represents one of the few nontrivial examples of a many-body quantum system for which a number of exact results have been obtained. The exact wave function, the ground state energy, the magnetic susceptibility at zero temperature, and the spectrum of triplet excitations have been determined. In the present article we shall determine the spectrum for arbitrary excitations and give their classification.

As is well known, the appropriate Hamiltonian has the form

$$H=\sum_{i=1}^{N-1}\left(\mathbf{S}_i\mathbf{S}_{i+1}-\frac{1}{4}\right)+\mathbf{S}_1\mathbf{S}_N-\frac{1}{4}. \tag{1}$$

Here the $\mathbf{S}_i$ are spin-$\frac{1}{2}$ operators.

In 1931 Bethe[1] was able to find the wave function for such a system. It has the following form for r reversed spins:

$$\Psi_r=\sum_{n_1,n_2,\dots,n_r=1}^{N}\Phi_r(n_1,n_2,\dots,n_r)S_{n_1}^+S_{n_2}^+\dots S_{n_r}^+|0\rangle, \tag{2}$$

$$\Phi_r(n_1,n_2,\dots,n_r)=\sum_{P=1}\exp\Big\{i\Big(\sum_{j=1}^{-}k_{P_j}n_j+\frac{1}{2}\sum_{j<i}\varphi_{P_iP_j}\Big)\Big\}, \tag{3}$$
$$n_1<n_2<\dots n_r.$$

The function $\Phi_r(n_1, n_2, \dots, n_r)$ is symmetric with respect to all n_i. The summation in (3) is over all permutations of the wave vectors k_i ($i = 1, 2, \dots, r$), P_j indicates the number produced at the location j as a result of the permutation P. The phases φ_{ij} satisfy the following equations:

$$Nk_j=2\pi\lambda_j+\sum_{l(\neq j)}\varphi_{jl}, \tag{4a}$$

$$2\operatorname{ctg}\frac{\varphi_{ij}}{2}=\operatorname{ctg}\frac{k_i}{2}-\operatorname{ctg}\frac{k_j}{2}. \tag{4b}$$

Here the λ_j are integers between 0 and $N-1$, and the φ_{ij} can be defined so that $-\pi<\operatorname{Re}\varphi_{ij}<\pi$. Finally the self-energy is expressed in the form

$$E=-\sum_{i=1}(1-\cos k_i). \tag{5}$$

Equation (4) was solved for a system of reversed spins of finite density in a number of articles.[2,3] In this connection it was assumed that the ground state of the system corresponds to real k_i. This assumption was rigorously proved in article[4]. Des Cloizeaux and Pearson[5] determined the triplet excitation spectrum corresponding to real k_i, and showed that it does not have a gap. Since the excitations of the type considered by des Cloizeaux and Pearson are related to a change in the number of reversed spins, it is necessary to classify them as Fermi excitations of the system. In this connection the singlet excitations (see Sec. 4), which are very important for a discussion of the temperature-dependent properties of such a chain and in applications to real systems, are in principle not included in them.

In order to obtain the spectrum of the boson-type excitations, it is necessary to leave the class of real k_i. Following Bethe we shall call states with complex k_i bound states. An analysis of the bound states for two reversed spins was given by Bethe[1] and Orbach[6] (in the case of a spin Hamiltonian with anisotropic coupling). In our article[7] the general case of L coupled reversed spins is considered (where L is finite, that is, $L \ll N$). Since this case is important for an understanding of the general classification of excited states in a system possessing a finite density of reversed spins, we give here an account of the results obtained in article[7].

2. SYSTEM WITH A FINITE NUMBER OF COUPLED SPINS

In order to solve Eqs. (4) for the case of a finite system of spins, let us assume that only the phases $\varphi_{12}, \varphi_{23}, \dots, \varphi_{L-1,L}$ are large. Later on this assumption will be given a rigorous foundation. Without any limitation in generality, we assume that $\operatorname{Im}\varphi_{l-1,l}>0$. Then from Eq. (4a) we have

$$\begin{aligned}\operatorname{Im}\varphi_{12}&=N\operatorname{Im}k_1=N\varkappa_1,\\ \operatorname{Im}(\varphi_{23}-\varphi_{12})&=N\operatorname{Im}k_2=N\varkappa_2,\\ &\dots\dots\dots\dots\\ -\operatorname{Im}\varphi_{L-1,L}&=N\operatorname{Im}k_L=N\varkappa_L.\end{aligned} \tag{6}$$

Note that we have chosen the phases so that

$$\sum_{i=1}^{l} \varkappa_i \geqslant 0 \text{ for all } l.$$

Substituting the larger phases into Eq. (4b), with an accuracy exponential in N we obtain

$$\operatorname{ctg}\frac{k_l}{2} = 2i + \operatorname{ctg}\frac{k_l - 1}{2}. \tag{7}$$

The solution of this system is obviously given by

$$\operatorname{ctg}(k_l/2) = 2li + C. \tag{8}$$

The constant C is determined in the following way. Let us introduce the total momentum of the spin system

$$u = \sum_{i=1}^{r} k_i = \sum_{i=1}^{r} \frac{2\pi}{N}\lambda_i.$$

In connection with the shift $n_i \to n_i + n$ the wave function $\psi_L(n_1 n_2 \ldots n_L)$ is multiplied by the factor $\exp(inu)$, where the energy levels are characterized by the momentum u. Taking this condition into account, we obtain the following expression for k_n:

$$e^{ik_n} = \frac{L - n(1 - e^{iu})}{L - (n-1)(1 - e^{iu})}, \quad n = 1, 2, \ldots, L. \tag{9}$$

In this connection for the energy we shall have

$$E_L(u) = -(1 - \cos u)/L. \tag{10}$$

This result agrees with the machine calculations of Bonner and Fisher,[8] carried out for a linear antiferromagnetic chain with N = 2, 3, ..., 11. The effective mass is proportional to L, just as one would expect. In order to convince oneself of the validity of the assumptions that have been made and in order to determine the set of integers λ_i for such a solution, it is necessary to carry out further analysis of Eqs. (4). First of all we note that the phases $\varphi_{n_1 n_2}$ of nonneighboring momenta ($|n_1 - n_2| \geq 2$) are pure imaginary and are actually small in comparison with the remaining phases. Using Eqs. (4b) and (8) we obtain

$$\varphi_{n_1 n_2} = i \ln \frac{n_1 - n_2 - 1}{n_1 - n_2 + 1}, \quad |n_1 - n_2| \geqslant 2. \tag{11}$$

Finally, in order to determine the λ_i let us write down the real parts of Eqs. (4a):

$$\begin{aligned} N \operatorname{Re} k_1 &= 2\pi\lambda_1 + \operatorname{Re}\varphi_{12}, \\ N \operatorname{Re} k_2 &= 2\pi\lambda_2 + \operatorname{Re}(\varphi_{23} - \varphi_{12}), \\ &\cdots\cdots\cdots\cdots \\ N \operatorname{Re} k_L &= 2\pi\lambda_L - \operatorname{Re}\varphi_{L-1,L}. \end{aligned} \tag{12}$$

The left-hand side of these equations is known from (9). For L even we have

$$\begin{gathered} \operatorname{Re} k_m = \operatorname{arctg}\frac{\eta}{L - 2m} - \operatorname{arctg}\frac{\eta}{L - 2m + 2} + \pi[1 - \varepsilon(\eta)], \\ m = 1, 2, \ldots, L/2 - 1; \\ \operatorname{Re} k_{L/2} = \frac{\pi}{2}\varepsilon(\eta) - \operatorname{arctg}\frac{\eta}{2} + \pi[1 - \varepsilon(\eta)]. \end{gathered} \tag{13}$$

Here $\eta = L \cot(u/2)$ and $\epsilon(\eta)$ is the sign function:

$$\begin{aligned} \varepsilon(\eta) &= 1 \quad \text{for} \quad \eta > 0, \\ \varepsilon(\eta) &= -1 \quad \text{for} \quad \eta < 0. \end{aligned}$$

The remaining k_m are determined from the condition

$$\operatorname{Re} k_m = \operatorname{Re} k_{L-m+1}, \tag{14}$$

which is satisfied for all L. For odd L we have

$$\begin{gathered} \operatorname{Re} k_m = \operatorname{arctg}\frac{\eta}{L - 2m} - \operatorname{arctg}\frac{\eta}{L - 2m + 2} + \pi[1 - \varepsilon(\eta)], \\ m = 1, 2, \ldots, (L-1)/2; \\ \operatorname{Re} k_{(L+1)/2} = \pi\varepsilon(\eta) - 2\operatorname{arctg}\eta + \pi[1 - \varepsilon(\eta)]. \end{gathered} \tag{15}$$

The remaining k_m are determined from (14).

Equations (12) for the λ_i and for the phases φ_{ij} can be solved in the following way. Let us consider the first equation of (12). If the fractional part $(N \operatorname{Re} k_1)/2\pi > 1/2$, then $-\operatorname{Re}\varphi_{12} > 0$ and it is chosen so as to bring the value of $N \operatorname{Re} k_1/2\pi$ up to an integer, and λ_1 will be exactly equal to this integer. If the fractional part $(N \operatorname{Re} k_1)/2\pi < 1/2$ then $-\operatorname{Re}\varphi_{12} < 0$ and it is chosen so as to decrease $N \operatorname{Re} k_1/2\pi$ to an integer value; λ_1 is equal to this integer.

The following phases $\varphi_{l-1,l}$ and λ_l are determined in similar fashion. For us it is essential here that this procedure gives the following result for $L \geq 3$:

$$\lambda_m = \lambda_{L-m+1}. \tag{16}$$

Here we exclude from consideration a certain number (small in comparison with N) of states for which the following exact equality accidentally holds: the fractional part $(N \operatorname{Re} k_1)/2\pi = 1/2$. In this case, for example, $\operatorname{Re}\varphi_{12}$ may be equal to either π or $-\pi$ and consequently $\lambda_1 = \lambda_L \pm 1$. Following Bethe,[1] we shall refer to states for which the latter equality holds as belonging to Category III, and states for which Eq. (16) is satisfied belong to Category II. States for which $|\lambda_i - \lambda_j| \geq 2$ belong to Category I. In this case the solution of the system of equations (4) corresponds to real momenta and phases.

For $L \geq 3$ the number of states belonging to Category II will be much larger (for large values of N) than the number of states belonging to Category III. In what follows the latter states will not play any role in our analysis. On the other hand, for L = 2 the number of states in Category II is approximately equal to the number of states in Category III. The case L = 2, however, was considered in sufficient detail in the articles by Bethe[1] and Orbach,[6] and in what follows we shall only use their results. Let us write down the further restrictions on u which follow from Eqs. (12)–(15). Summing over all k_m we obtain

$$u = \sum_{m=1}^{L} k_m = \pi\varepsilon(\eta) - 2\operatorname{arctg}\frac{\eta}{L} + L\pi[1 - \varepsilon(\eta)]. \tag{17}$$

This last equality is an identity only in that case when

$$0 < u < \pi \text{ and } (2L-1)\pi < u < 2L\pi. \tag{18}$$

Now it only remains to verify the assumed positiveness of $\operatorname{Im}\varphi_{l,l+1}$. Using (6) and (9) we obtain (for $l < L$):

$$\begin{aligned} |\exp\{i\varphi_{l,l+1}\}|^2 &= \exp\{-2(\varkappa_1 + \varkappa_2 + \ldots + \varkappa_l)\} \\ &= 1 - \frac{4l}{L}\left(1 - \frac{l}{L}\right)\sin^2\frac{u}{2} \leqslant 1, \end{aligned} \tag{19}$$

which also justifies the assumption made.

We note that the entire calculation has been made with an accuracy exponential in N; therefore it is no wonder that the numerical calculations of Bonner and Fisher[8] for N = 2, 3, ..., 11 are approximated well by expression (10). The few states for which $u \sim 0$ or 2π constitute an exception since in this case the phases $\varphi_{l,l-1}$ chosen by us are not large, and our solution is not applicable.

3. BOUND STATES FOR A SYSTEM OF N/2 REVERSED SPINS[1)]

Before going on to a determination of the excited states with $S_z = 0$, let us present the results of a solution of the system of equations (4) for the ground state.[1,2] As shown in[4], the ground state of the system belongs to Category I. In this case $\lambda_i = 2i - 1$ $(i = 1, 2, \ldots, N/2)$ and a solution of the system of equations (4) exists such that all momenta and phases are real. For the latter we have the expression

$$\varphi_{ij} = \pi\varepsilon(\xi_i - \xi_j) - 2\,\mathrm{arctg}\,\frac{\xi_i - \xi_j}{2}. \tag{20}$$

Here $\xi_i = \cot(k_i/2)$. One can represent Eq. (4a) in the following form:

$$\frac{\pi}{2} - 2\,\mathrm{arctg}\,\xi_i = \frac{\pi(2i-1)}{N} - \frac{2}{N}\sum_{j=1}^{N/2}\mathrm{arctg}\,\frac{\xi_i - \xi_j}{2}. \tag{21}$$

Changing to a continuous distribution of the quantities ξ_i, one can obtain the Hulthén equation for their density $\rho_0(\xi)$:

$$\rho_0(\xi) + \frac{2}{\pi}\int_{-\infty}^{\infty}\frac{d\xi'\rho_0(\xi')}{4 + (\xi - \xi')^2} = \frac{2}{\pi(1+\xi^2)}, \tag{22}$$

which is easily solved by Fourier transform. The ground state energy is expressed in terms of the function $\rho_0(\xi)$ in the following way:

$$E_0 = -\sum_{i=1}^{N/2}\frac{2}{1+\xi_i^2} = -N\int_{-\infty}^{\infty}\frac{\rho_0(\xi)}{1+\xi^2}\,d\xi. \tag{23}$$

It is easy to show that if one chooses

$$\xi_i = \frac{2}{\pi}\ln\mathrm{ctg}\,\frac{\pi(2i-1)}{2N}, \quad i = 1, 2, \ldots, N/2, \tag{24}$$

then the entire calculation, including the transition to a continuous distribution, will be valid to within $1/N^2$. This is also confirmed by the numerical calculations in[8]. For example, for finite N the ground state energy is well-approximated by an expression of the form $E_N = E_0 + (a/N^2)$ (terms $\sim 1/N$ are not present).

The excited states belonging to Category I are determined in the following way.[5] A set of integers λ_i is chosen in the form: $\lambda_i = 0, 2, 4, \ldots, 2n-2, 2n+1, \ldots, N-1$. In this connection it is found that $k_1 = 0$, and the remaining $(N/2) - 1$ momenta are real and have a distribution close to $\rho_0(\xi)$:[5]

$$\rho_1(\xi) = \rho_0(\xi) - 2N^{-1}R(\xi, \xi_0),$$
$$\rho_0(\xi) = \left(2\,\mathrm{ch}\,\frac{\pi\xi}{2}\right)^{-1}, \quad \mathrm{sh}\,\frac{\pi\xi_0}{2} = \mathrm{ctg}\,\frac{2\pi n}{N}. \tag{25}$$

In this connection the excitation energy is given by

$$\varepsilon_{tr}(q) = {}^1\!/_2\pi|\sin q|. \tag{26}$$

The spin of such excitations is $S = 1$, and $q = 2\pi n/N$ is the total momentum of the system.

In order to determine the excited bound states of a system of N/2 reversed spins ($S_z = 0$) we note that the system of equations for the phases φ_{ij} and for the momenta k_i possesses the following properties. Let, for example, there by two complex conjugate momenta k_a and k_b ($k_a^* = k_b$) among the system of momenta, and let all remaining momenta k_i be real. We shall demonstrate that this does not contradict the system of equations (4) if $\lambda_a = \lambda_b$ or $\lambda_a = \lambda_b \pm 1$. Actually, from (4b) one can easily see that $\varphi^*(k_a, k_i) = \varphi(k_b, k_i)$ and $\varphi(k_a, k_b)$ is either pure imaginary (for $\lambda_a = \lambda_b$) or has a real part equal to $\pm\pi$ (for $\lambda_a = \lambda_b \pm 1$).

The equation for k_a has the following form:

$$Nk_a = 2\pi\lambda_a + \sum_i \varphi(k_a, k_i) + \varphi(k_a, k_b). \tag{27}$$

By taking the complex-conjugate of this equation we obtain an equation for k_b. Finally, the remaining equations from (4a) for k_i do not contradict the fact that the k_i are real:

$$Nk_i = 2\pi\lambda_i + \sum_j \varphi_{ij} + (\varphi_{ia} + \varphi_{ib}),$$

since $\varphi_{ia} + \varphi_{ib}$ is real. Similarly, one can show that the presence of several complex-conjugate pairs of momenta, with all remaining momenta being real, also does not contradict the basic equations. Moreover, as Bethe showed, in order for the latter to be real the corresponding λ_i must satisfy the inequality $|\lambda_i - \lambda_j \geq 2$. So we require $|\lambda_i - \lambda_{a,b}| \geq 2$.

Using this property, let us divide all momenta into complex momenta, which we shall label with indices m, m' $(m = 1, 2, \ldots, L)$, and into real momenta which we shall label by indices i, j $(i = 1, \ldots, N/2 - L)$. In terms of this notation the fundamental equations (4a) and (4b) are rewritten in the following form:

$$Nk_i = 2\pi\lambda_i + \sum_j \varphi_{ij} + \sum_{m=1}^{L}\varphi_{im}, \tag{28a}$$

$$Nk_m = 2\pi\lambda_m + \sum_j \varphi_{mj} + \sum_{m'}\varphi_{mm'}, \tag{28b}$$

$$2\,\mathrm{ctg}\,\frac{\varphi_{ij}}{2} = \mathrm{ctg}\,\frac{k_i}{2} - \mathrm{ctg}\,\frac{k_j}{2}, \tag{29a}$$

$$2\,\mathrm{ctg}\,\frac{\varphi_{im}}{2} = \mathrm{ctg}\,\frac{k_i}{2} - \mathrm{ctg}\,\frac{k_m}{2}, \tag{29b}$$

$$2\,\mathrm{ctg}\,\frac{\varphi_{m,m'}}{2} = \mathrm{ctg}\,\frac{k_m}{2} - \mathrm{ctg}\,\frac{k_{m'}}{2}. \tag{29c}$$

Let us consider the last equation, (29c). If one again (see Sec. 2) assumes that only the phases $\varphi_{m-1,m}$ are large, where $-\mathrm{Im}\,\varphi_{m,m-1} \sim N$ and greater than zero, then one can easily obtain an expression for k_m analogous to (9). Then we have

$$e^{ik_m} = \frac{L - m(1 - e^{i\bar{u}})}{L - (m-1)(1 - e^{i\;})}, \quad \bar{u} \quad \sum_{m=1}^{L} k_m. \tag{30}$$

Using (30) we obtain an expression for the mixed phases φ_{im}, where only their real part is required for our purposes. Omitting the lengthy calculations, we obtain the following result for even L:

$$\mathrm{Re}\,\varphi_{im} = \mathrm{arctg}\,\frac{\bar{\eta} - \xi_i}{L + 3 - 2m} - \mathrm{arctg}\,\frac{\bar{\eta} - \xi_i}{L - 1 - 2m}, \quad m = 1, 2, \ldots, \frac{L}{2} - 1,$$

$$\mathrm{Re}\,\varphi_{i,L/2} = \mathrm{arctg}\,\frac{\bar{\eta} - \xi_i}{2} + \mathrm{arctg}\,(\bar{\eta} - \xi_i) - \pi\varepsilon(\bar{\eta} - \xi_i). \tag{31}$$

Here $\xi_i = \cot(k_i/2)$ and $\bar{\eta} = L\cot(\bar{u}/2)$. For L odd we have

$$\mathrm{Re}\,\varphi_{im} = \mathrm{arctg}\,\frac{\bar{\eta} - \xi_i}{L + 3 - 2m} - \mathrm{arctg}\,\frac{\bar{\eta} - \xi_i}{L - 1 - 2m}, \quad m = 1, \ldots, \frac{L-3}{2},$$

$$\mathrm{Re}\,\varphi_{i,(L-1)/2} = \mathrm{arctg}\,\frac{\bar{\eta} - \xi_i}{4} - \frac{\pi}{2}\varepsilon(\bar{\eta} - \xi_i),$$

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1)We shall assume that N is even.

$$\operatorname{Re}\varphi_{i,(L+1)/2} = 2\operatorname{arctg}\frac{\bar{\eta}-\xi_i}{2} - \pi\varepsilon(\bar{\eta}-\xi_i). \qquad (32)$$

Substituting these expressions for the mixed phases into (28b), let us determine the λ_m corresponding to such k_m. In this connection in order to determine λ_m it is necessary for us to know ξ_i or their distribution on the real axis. Assuming that to zero order in N this distribution coincides with $\rho_0(\xi)$, i.e., with their distribution in the ground state, we find an expression for λ_m which is finite, to within a few ($\sim L$) units. Carrying out the corresponding calculations to zero order in N, we obtain the following results for L even:

$$\operatorname{Re}k_m = \frac{2\pi\lambda_m}{N} + \operatorname{arctg}\frac{\bar{\eta}}{L-2m} - \operatorname{arctg}\frac{\bar{\eta}}{L-2m+2},\ m = 1,\ldots,\frac{L}{2}-1,$$

$$\operatorname{Re}k_{L/2} = \frac{2\pi\lambda_{L/2}}{N} - \operatorname{arctg}\frac{\bar{\eta}}{2} - \frac{\pi}{2} + 2\operatorname{arctg}e^{\pi\bar{\eta}/2}, \qquad (33)$$

and for L odd we find

$$\operatorname{Re}k_m = \frac{2\pi\lambda_m}{N} + \operatorname{arctg}\frac{\bar{\eta}}{L-2m} - \operatorname{arctg}\frac{\bar{\eta}}{L-2m+2},\ m = 1,\ldots,\frac{L-1}{2}$$

$$\operatorname{Re}k_{(L+1)/2} = \frac{2\pi}{N}\lambda_{(L+1)/2} - 2\operatorname{arctg}\bar{\eta} + 2\,[2\operatorname{arctg}e^{\pi\bar{\eta}/2} - \pi/2]. \qquad (34)$$

If the results for k_m obtained in the preceding Section (formulas (13)–(15)) are used, then from (33) and (34) one can easily reach the following conclusions. All λ_m with the exception of $\lambda_{L/2}$ and $\lambda_{L/2+1}$ for even L and $\lambda_{(L+1)/2}$ for odd L are grouped around zero if $\bar{\eta} > 0$ or around N if $\bar{\eta} < 0$. For $\lambda_{L/2}, \lambda_{L/2+1}$, and $\lambda_{(L+1)/2}$[2)] we have:

$$\frac{2\pi\lambda_{L/2}}{N} = \frac{2\pi\lambda_{L/2+1}}{N} = \pi - 2\operatorname{arctg}e^{\pi\bar{\eta}/2} + \frac{\pi}{2}(1-\varepsilon(\bar{\eta})),$$
$$\frac{2\pi\lambda_{(L+1)/2}}{N} = 2\pi - 4\operatorname{arctg}e^{\pi\bar{\eta}/2}. \qquad (35)$$

This information about λ_m is sufficient to determine the numbers ξ_i or, more precisely, to determine their distribution function, which one needs in order to calculate the excitation energy. To this end and let us return to Eq. (28a). In order to make this expression closed, it is necessary to choose the numbers λ_i. This choice is limited by the following conditions:

$$|\lambda_i - \lambda_j| \geqslant 2, \qquad |\lambda_i - \lambda_m| \geqslant 2,$$

in this connection a solution of Eqs. (28a) must exist for which all k_i are real, $k_i \neq k_j$ for $i \neq j$ and all $k_i \neq 0$ or 2π.

Let us illustrate the choice of λ_i for the example L = 2 or 3. First let L = 2. Let us add two real momenta k_{i_1} and k_{i_2} (we may label the momenta arbitrarily) to a system consisting of (N/2) − 2 momenta k_i. In this connection we shall assume that the supplemented system of momenta satisfies a modified system of equations

$$Nk_i = 2\pi\lambda_i + \sum_{j=1}^{N/2}\varphi_{ij} - \varphi_{ii_1} - \varphi_{ii_2} + \sum_{m=1}^{2}\varphi_{im}, \quad i = 1, 2, \ldots, N/2. \ (36)$$

We shall assume that $\varphi_{ii} = 0$. It is easy to see that this system decomposes into (N/2) − 2 equations like (28a) and two equations for the additional momenta k_{i_1} and k_{i_2}. Our next step will be to choose the λ_i just as for the ground state, $\lambda_i = 2i - 1$ ($i = 1, 2, \ldots, N/2$). In this connection i_1 (or i_2) is chosen from the condition $\lambda_{i_1} = \lambda_{L/2} = \lambda_{L/2+1}$ (L = 2) since among the numbers λ_i in Eq. (28a) there cannot be any equal to $\lambda_{L/2}$ (according to the requirement $|\lambda_i - \lambda_m| \geq 2$). Using (35) this can be rewritten in the form

$$\frac{2\pi}{N}(2i_1 - 1) = \pi - 2\operatorname{arctg}e^{\pi\bar{\eta}/2} + \frac{\pi}{2}[1-\varepsilon(\bar{\eta})]. \qquad (37)$$

At first glance there is complete freedom in the choice of i_2. However, it turns out that one can prove an existence theorem for the solutions of the system of equations (28a) (with given λ_i) only in that case when (see Appendix)

$$\operatorname{ctg}(k_{i_2}/2) \cong \bar{\eta}. \qquad (38)$$

For L = 3 it is also necessary to construct a modified system of equations of the type (36). It will contain three additional momenta, k_{i_1}, k_{i_2}, and k_{i_3}. Just as in the previous case, let us choose $\lambda_i = 2i - 1$. Then i_1, i_2, and i_3 are determined in the following way: i_1 and i_2 are chosen from the conditions $\lambda_{i_1} = \lambda_{(L+1)/2}$ and $\lambda_{i_2} = \lambda_{(L+3)/2}$ since among the numbers λ_i in Eq. (28a) no numbers equal to $\lambda_{(L+1)/2}$ or $\lambda_{(L-1)/2}$ can occur. This indicates that i_2 is close to zero or N/2, and from (35) we have the following result for i_1

$$2\pi(2i_1 - 1)/N = 2\pi - 4\operatorname{arctg}e^{\pi\bar{\eta}/2}. \qquad (37')$$

The number i_3 is again chosen so that a solution exists for the system of equations (28a); it turns out that for this it is necessary that

$$i_3 = i_1 \pm 1. \qquad (38')$$

In the case of values of L greater than three, it is also necessary to write down a modified system of equations. It will have the form

$$Nk_i = 2\pi\lambda_i + \sum_{j=1}^{N/2}\varphi_{ij} + \sum_{m=1}^{L}\varphi_{im} - \sum_{k=1}^{L}\varphi_{ii_k}, \qquad (39)$$
$$\lambda_i = 2i - 1, \quad i = 1, 2, \ldots, N/2.$$

We introduced L additional momenta k_{i_1}, $k_{i_2}, \ldots, k_{i_L}$ and L supplementary equations. The choice of the two numbers i_1 and i_2 for even L and of the three numbers i_1, i_2, and i_3 for odd L is made with the aid of the same equations (37), (38), (37′), and (38′). The remaining numbers of this series are determined either with the aid of (33) and (34) or else from the fact that we are considering the lowest bound-type excitation with a given L and total momentum

$$Q = \frac{2\pi}{N}\sum_{i=1}^{N/2}\lambda_i.$$

In this connection the remaining i_k turn out to be close to either zero or N/2.

A formal solution of the modified system (39) is obtained in the following way. First of all let us rewrite this system in terms of ξ_i:

$$\frac{\pi}{2} - 2\operatorname{arctg}\xi_i = \frac{\pi(2i-1)}{N} - \frac{2}{N}\sum_{j=1}^{N/2}\operatorname{arctg}\frac{\xi_i - \xi_j}{2} + \frac{T(\xi_i)}{N},$$

2) $\lambda_{L/2}$ and $\lambda_{L/2+1}$ for even L; $\lambda_{(L+1)/2}$ for odd L.

$$T(\xi_i)=2\pi\varepsilon(\xi_i-\bar{\eta})-2\,\mathrm{arctg}\frac{\xi_i-\bar{\eta}}{L+1}-2\mathrm{arctg}\frac{\xi_i-\bar{\eta}}{L-1}+$$
$$+\sum_{m=1}^{L}\left\{2\,\mathrm{arctg}\frac{\xi_i-\bar{\xi}_m}{2}-\pi\varepsilon(\xi_i-\bar{\xi}_m)\right\},\qquad (40)$$

ξ_m is expressed in terms of the additional momenta in the usual way. The transition to a continuous variable is achieved by differentiation of both parts of the equation with respect to ξ_i and by the introduction of the density of the distribution of the numbers ξ_i with the aid of the formal equation

$$\rho(\xi)=-\frac{2}{N}\frac{di}{d\xi_i}.\qquad (41)$$

In this connection the equation for $\rho(\xi)$ takes the form

$$\rho(\xi)+\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{2\rho(\xi')}{4+(\xi-\xi')^2}d\xi'=\frac{2}{\pi(1+\xi^2)}+\frac{1}{\pi N}\frac{dT(\xi)}{d\xi}$$
$$\frac{dT}{d\xi}=4\pi\delta(\xi-\bar{\eta})-\frac{2(L+1)}{(L+1)^2+(\xi-\bar{\eta})^2}-\frac{2(L-1)}{(L-1)^2+(\xi-\bar{\eta})^2}+$$
$$+\sum_{m=1}^{L}\left[\frac{4}{4+(\xi-\bar{\xi}_m)^2}-2\pi\delta(\xi-\bar{\xi}_m)\right].\qquad (42)$$

Introducing the Fourier transform of the function $\rho(\xi)$ according to the formula

$$\tilde{\rho}(k)=\int_{-\infty}e^{ik\xi}\rho(\xi)\,d\xi$$

and taking the Fourier transform over the entire equation (42), we obtain

$$\tilde{\rho}(k)=\frac{1}{\mathrm{ch}\,k}+\frac{2}{N}e^{|k|}\frac{1}{\mathrm{ch}\,k}(1-e^{-L|k|}\,\mathrm{ch}\,k)e^{i\bar{\eta}k}$$
$$-\frac{2}{N}\mathrm{th}|k|\sum_{m=1}^{L}e^{i\bar{\xi}_m k}.\qquad (43)$$

It is convenient to rewrite expression (23) for the energy in the following way:

$$E=-\sum_{i=1}^{N/2}\frac{2}{1+\xi_i^2}+\sum_{m=1}^{L}\left(\frac{2}{1+\bar{\xi}_m^2}-\frac{2}{1+\xi_m^2}\right).\qquad (44)$$

Here we have subtracted and added the sum over the additional momenta. Changing to a continuous variable ξ and performing an integration with the function $\rho(\xi)$, we obtain an interesting expression for the energy of an excited bound-type state

$$E=E_0-\pi/\mathrm{ch}\frac{\pi\bar{\eta}}{2}+\sum_{m=1}^{L}\pi/\mathrm{ch}\frac{\pi\bar{\xi}_m}{2}.\qquad (45)$$

Here $E_0 = -N\ln 2$, the well known expression for the energy of the ground state of an antiferromagnetic chain.[2]. In order to determine the energy of the lowest excited state possessing total momentum Q, it is necessary to utilize the system of equations (37), (37′), (38), (38′), and (24), and also the fact that for the lowest excited state it is necessary to set the free $\bar{\xi}_m$ equal to $\pm\infty$. Taking this into consideration, one can easily obtain the following expression[3)] (for all L) for the excitation energy $\epsilon_L(q)$:

$$\varepsilon_L(q)=\pi|\sin(q/2)|,\quad -\pi/2<q<\pi/2.\qquad (46)$$

Here $q = Q - Q_0$ where Q_0 is the momentum of the ground state. It is remarkable that the spectrum of the lowest bound-type excitations does not depend on L. Of course, higher excitations of a combined type exist when several excitations from Category II are present in the system together with excitations from Category I. Finally, from (46) it follows that the bound excited states also do not have a gap in their excitation spectrum.

4. TOTAL SPIN OF THE EXCITED STATES

By direct action of the operator $\hat{S}^2$ on the wave function (3) one can easily verify that upon fulfilment of Eqs. (4a) and (6) it is an eigenfunction of the total spin operator, and also

$$S=\left|\frac{N}{2}-r\right|+M=|S_z|+M,\quad M<r,\qquad (47)$$

where r is the number of reversed spins and M is the number of momenta k_j which are equal to zero. From this expression it follows, for example, that S = 0 for the ground state, and the excited states belonging to Category I always have nonvanishing spins. However, bound states of the type described by us have S = 0.

APPENDIX

Let us present a proof of the existence of solutions of the system of equations (28a) for L = 2.

Following Griffiths,[3] we shall regard Eq. (28a) as a nonlinear transformation $\hat{D}$ of a vector **k** with components $(k_1, k_2, \ldots, k_{i_1-1}, k_{i_1+1}, \ldots, k_{N/2})$ into a new vector **k**′:

$$k_i'=\hat{D}k_i=\frac{2\pi\lambda_i}{N}+\frac{1}{N}\sum_{j(\neq i_1 i_2)}\varphi(k_i,k_j)+\sum_{m=1}^{2}\varphi(k_i,k_m).\qquad (A.1)$$

Here $\lambda_i = 2i - 1$, i_1, and i_2[4)] are determined with the aid of the system of equations (37), (38), and (24). The solution of Eq. (39) represents a fixed point of this transformation. We shall show that if the transformation $\hat{D}$ is carried out on a vector **k** with the following properties

$$k_1\geqslant\frac{2\pi}{N},\quad k_{N/2}\leqslant 2\pi\left(1-\frac{1}{N}\right),\qquad (A.2)$$
$$k_{j+1}-k_j\geqslant 2\pi/N,\quad j=1,2,\ldots,i_2-1,i_2+1,\ldots,N/2-1,$$

and also

$$k_{i_2+1}-k_{i_2-1}\geqslant 2\pi/N,\qquad (A.3)$$

then the transformed vector **k**′ possesses the same properties. Actually

$$k_{j+1}'-k_j'\geqslant\frac{4\pi}{N}-\frac{2}{N}\varphi(k_j,k_{j+1})\geqslant\frac{2\pi}{N}\qquad (A.4)$$

for all j except $j = i_2, i_2 - 1$. Here we have used the fact that the function $\varphi(k_i, k_j)$ is positive for $k_j > k_i$, negative for $k_i > k_j$, and is an increasing function of k_i everywhere with the exception of the point of discontinuity, $k_i = k_j$. The function $\varphi_{i1} + \varphi_{i2}$ is also increasing with respect to k_i. An exception is the point of discontinuity of $\varphi_{i1} + \varphi_{i2}$, obtained from Eq. (40):

$$\mathrm{ctg}\frac{k_i}{2}=\bar{\eta}.$$

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3)For convenience the answer is reduced to the interval $-\pi < q < \pi$.

4)We shall assume that $\xi_{i_2+1} < \bar{\eta} < \xi_{i_2-1}$.

Near this point, however, we have

$$k'_{i_2+1} - k'_{i_2-1} \geqslant \frac{8\pi}{N} - \frac{2}{N}\varphi(k_{i_2-1}, k_{i_2+1}) + \sum_{m=1}^{2}[\varphi(k_{i_2-1}, k_m) - \varphi(k_{i_2+1}, k_m)] \geqslant \frac{2\pi}{N}, \qquad \text{(A.5)}$$

which also proves the assertion which has been made.

We cannot immediately use the theorem about a fized point since for arbitrary $\overline{\eta}$ the nonlinear transformation **D** is not continuous (because of the term $\varphi_{i_1} + \varphi_{i_2}$). If, however, the fact that

$$2\operatorname{arc\,ctg}\overline{\eta} = k_{i_2+1} - x,$$

is considered, then for arbitrary x satisfying the inequality $0 < x < 2\pi/N$ the transformation $\hat{\mathbf{D}}$ becomes continuous, and according to the theorem about a fixed point the system (28a) will have a solution. Later on it is necessary to choose the value of x so that Eq. (28a) is satisfied. We note that if ξ_{i_2} is not close to η, inequality (A.4) is not satisfied, and the proof does not go through. The proof is easily extended to large values of L.

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