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The Spin-Wave Continuum of the $S = 1/2$ Linear Heisenberg Antiferromagnet

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In the $S = 1/2$ linear Heisenberg antiferromagnet (HB AF)

$$H = J\sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1} - h\sum_{i=1}^{N} S_i^z \tag{1}$$

– although investigated by various theoretical approaches – many important questions concerning the statics and the dynamics have remained open. Recent low-temperature neutron- scattering experiments on $\mathrm{CuCl_2 \cdot 2N(C_5H_5)}$ (CPC) , which is a good realization of an $S = 1/2$ HB AF chain, provided new important information on the dynamics of the system, such as lineshapes and the behaviour in a magnetic field [1]. The important quantity for direct comparison with experiments of this kind is the dynamic spin-correlation function in (q,ω)-space. It is the Fourier transform of $\langle S^z(l,t)S^z(l',0)\rangle$, and for $T = 0$ it can be written as

$$G_{zz}(q,\omega) = \sum_{\lambda} M_\lambda \delta\big(\omega + E_0 E_\lambda\big), \quad M_\lambda = 2\pi |\langle 0|S^z(q)|\lambda|^2. \tag{2}$$

In a recent publication [2] an approximate analytical expression for G_{zz}G at $T = 0$ and $h = 0$ was obtained by using finite-chain calculations together with the results of two other theoretical approaches. It represents the dominant contribution to $G_{zz}(q,\omega)$ originating from a spin-wave continuum (SWC) bounded between the dispersion branches $E_1(q) = (\pi J/2)|\sin q|$ and $E_2(q) = \pi J|\sin(q/2)|$:

$$G_{zz}^{\mathrm{SWC}}(q,\omega) = 2\big\{\omega^2 - [E_1(q)]^2\big\}^{-1/2}\theta\big(\omega - E_1(q)\big)\theta\big(E_2(q) - \omega\big). \tag{3}$$

G_{zz} increases strongly towards the lower bound $E_1(q)$, which is the desCloizeaux-Pearson spin-wave energy. Result (3) is in good agreement with experimental data for CPC concerning excitation energy, lineshape and integrated intensity [1,2].

In this note we give further arguments supporting (3), which demonstrates the usefulness of finite-chain calculations for properties of the infinite system. Although we cannot give a rigorous derivation of (3), we conjecture that it represents the SWC quantatively. We have identified those excitations of the finite system which have dominant spectral weight with a special class of eigenstates in the Bethe formalism [3], and we show that these states form, in the thermodynamic limit, a continuum exactly between the two branches $E_1(q)$ and $E_2(q)$. The Bethe Ansatz for the exact eigenfunctions consists of a linear combination $\psi = \sum a(n_1,\ldots,n_r)\phi(n_1,\ldots,n_r)$ of local basis vectors with reversed spins at lattice sites $n_1,\ldots,n_r$ with coefficients of the form

$$a(n_1,\ldots,n_r) = \sum_p \exp\left(\mathrm{i}\sum_j k_{p_j} n_j + \frac{1}{2}\mathrm{i}\sum_{j<l}\psi_{p_j p_l}\right), \tag{4}$$

where the summation $\sum_p$ extends over all permutations of the integers $1, \ldots, r$ and p_j is the image of j under the pth permutation. The k_j and the ψ_{ij} obey the coupled equations:

$$2 \cot \frac{\psi_{jl}}{2} = \cot \frac{k_j}{2} - \cot \frac{k_l}{2}, \quad N k_j = 2\pi\lambda_j + \sum_{l \neq j} \psi_{jl}. \tag{5}$$

The integers λ_j are confined to $1 \leq \lambda_j \leq N-1$, and each choice of a set $\{\lambda_j\}$ (being subject to additional restrictions) determines an eigenstate of the system. Having solved the above equations for k_j, it is straightforward to calculate wave number and energy of the corresponding eigenstate,

$$q = \sum_{j=1}^{r} k_j = \frac{2\pi}{N} \sum_{j=1}^{r} \lambda_j, \quad E = -\sum_{j=1}^{r} (1 - \cos k_j). \tag{6}$$

The ground state, which is a singlet (for even N), corresponds to the $N/2$ integers $\lambda_j = 1, 3, 5, \ldots,$ $(N-1)$. Des Cloizeaux and Pearson [4] found the lowest excited states to be given by

$$\begin{array}{ll} 1, 3, \ldots, (N-2n-1), (N-2n+2), \ldots, (N-2) & q > 0 \\ 2, 4, \ldots, (2n-2), (2n+1), \ldots, (N-1) & q < 0 \end{array} \tag{7}$$

($q = 2\pi n/N$) and calculated their energies. The result is the famous DC-P spin-wave branch $E_1(q)$. By generalization of their method we have found the sets $\{\lambda_j\}$ for all SWC states. To the highest branch $E_2(q)$, in particular, belong the sets (always for even N):

$$\begin{array}{ll} 1, 3, \ldots, (N-n-2), (N-n+2), \ldots, (N-1) & n \text{ odd} \\ 1, 3, \ldots, (N-n-3), (N-n), (N-n+3), \ldots, (N-1) & n \text{ even} \end{array} \tag{8a}$$

for $q > 0$ and

$$\begin{array}{ll} 1, 3, \ldots, (n-2), (n+2), \ldots, (N-1) & n \text{ odd} \\ 1, 3, \ldots, (n-3), n, (n+3), \ldots, (N-1) & n \text{ even} \end{array} \tag{8b}$$

for $q < 0$. Using these numbers we can calculate (in the thermodynamic limit) the energies of all the excitations of the two-parameter SWC ($q > 0$ for convenience):

$$E_b(q) = \pi J \left| \sin \frac{q}{2} \cos \left(\frac{q}{2} - \frac{q_b}{2} \right) \right|, \tag{9}$$

where q ($0 \leq q \leq \pi$) is the wave number of the excitation (now with respect to that of the ground state) and q_b ($0 \leq q_b \leq q$) labels the different dispersion branches within the continuum. The lowest branch $E_1(q)$ has $q_b = 0$ and the highest one has $q_b = q$ yielding $E_2(q)$. Furthermore (9) immediately provides the density of states in the SWC

$$D(q, \omega) = \frac{N}{2\pi} \left\{ \left[E_2(q) \right]^2 - \omega^2 \right\}^{-1/2} \tag{10}$$

According to (2) $G_{zz}^{\mathrm{SWC}}(q, \omega)$ is the product of the density of states $D(q, \omega)$ and a spectral weight defined by the squared matrix elements between the ground state and the SWC excitations: $M(q, \omega) \equiv |\langle 0, 0 | S^z(q) | \omega, q \rangle|^2$, yielding

$$M(q, \omega) = \frac{4\pi}{N} \sqrt{\frac{\left[E_2(q) \right]^2 - \omega^2}{\omega^2 - \left[E_1(q) \right]^2}}. \tag{11}$$

Comparison of (11) with finite-chain matrix elements shows good agreement.

This approach to the dynamics of the $S = 1/2$ HB AF at $T = 0$ can be extended to the $h \neq 0$ case. From finite-chain calculations we have determined the excitations contributing significantly to $G_{zz}(q,\omega)$. Again we have identified this class of excitations unambiguously with a certain class of eigenstates in the Bethe formalism. The calculations to solve eq's (5) for these states are in progress. Preliminary approximate results show that $G_{zz}(q,\omega)$ is dominated by two partly overlapping continua of excitations. Fig. 1 shows the boundaries of these continua for a special value of h. Again, the spectral weight of $G_{zz}(q,\omega)$ increases strongly as the frequency is lowered towards the lower boundary of each continuum. Further we find that $G_{xx}(q,\omega)$ looks for $h \neq 0$ qualitatively different from $G_{zz}(q,\omega)$. In particular, the lowest branch is inverted with respect to the axis $q = \pi/2$. Therefore we expect appropriate neutron scattering experiments to show spectra which are more complex than for $h = 0$ (having at least two dominant peaks), and which strongly depend on the relative weight of G_{xx} and G_{zz} in the scans under consideration. More details will be published elsewhere.

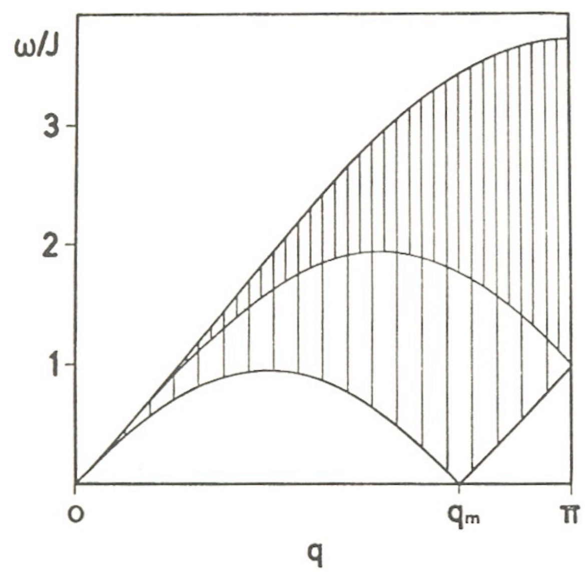

Figure 1. The two continua of excitations dominating $G_{zz}(q,\omega)$ at $T = 0$ and $h = \frac{1}{2}h_{\text{crit}}$. In each continuum the spectral weight increases strongly towards the corresponding lower boundary. The lowest boundary corresponds approximately to the spin-wave frequency obtained numerically by Ishimura and Shiba [5] and to the approximate analytical result by Pytte [6]. The special wave number q_m depends only on the magnetization. It is equal to π at $h = 0$ and decreases as h increases, reaching zero at the critical field h_{crit}.

Acknowledgments

We have used a modified cmpj.sty style file.

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