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Zero-Temperature Dynamics of the $s = \frac{1}{2}$ Linear Heisenberg Antiferromagnet in a Magnetic Field

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Analytic calculations in the Bethe formalism and finite-chain calculations show that the dynamic spin-correlation function in (q, ω) -space of the $s = \frac{1}{2}$ linear Heisenberg antiferromagnet at $T = 0$ in a uniform magnetic field is governed by a double continuum of excitations. Appropriate neutron scattering experiments are expected to show double-peak spectra.

We study the one-dimensional $s = \frac{1}{2}$ antiferromagnet in a magnetic field h with Hamiltonian

$$\mathcal{H} = \sum_{l=1}^N \mathbf{S}(l) \cdot \mathbf{S}(l+1) - h \sum_{l=1}^N S_z(l). \quad (1)$$

Various quasi one-dimensional magnets, such as CPC [1], can be described by this Hamiltonian for temperatures above their 3-d ordering temperature. We are interested in the dynamic spin correlation functions in (q, ω) -space, which are measured by inelastic neutron scattering:

$$G_{\alpha\alpha}(q, \omega) = \int dt e^{i\omega t} \sum_l e^{iq l} \langle S_\alpha(l, t) S_\alpha(0, 0) \rangle. \quad (2)$$

At $T = 0$

$$G_{\alpha\alpha}(q, \omega) = 2\pi \sum_\lambda |\langle 0 | S_\alpha(q) | \lambda \rangle|^2 \delta(\omega + E_0 - E_\lambda). \quad (3)$$

Since, even at $T = 0$, an exact solution for $G_{\alpha\alpha}$ is not easily available we aim at an approximate analytical expression, which represents $G_{\alpha\alpha}(q, \omega)$ as accurately as possible. In two recent papers [2, 3] we used the following arguments for $h = 0$. (i) Finite-chain calculations show that among the eigenstates $|\lambda\rangle$ which contribute to (3), those with total spin $S_T = 1$ belonging to the so-called spin wave continuum (SWC) are by far the most important. The corresponding matrix elements become very large for energies close to the lower edge of the SWC. (ii) Bethe's formalism for the eigenstates of (1) yields exact expressions for the lower and the upper boundaries of the SWC:

$$E_L(q) = \frac{\pi}{2} |\sin q|, \quad E_U(q) = \pi \left| \sin \frac{q}{2} \right|.$$

(iii) Calculations in the framework of a continuum model for interacting fermions [4] yield rigorous results for low frequencies at $q \simeq 0$ and $q \simeq \pi$.

All this suggests that G_{zz} ($= G_{xx} = G_{yy}$) be approximated by

$$G_{zz}(q, \omega) = 2[\omega^2 - E_L^2(q)]^{-1/2} \Theta(\omega - E_L(q)) \Theta(E_U(q) - \omega). \quad (4)$$

Implications of this form have been checked by calculating various static quantities in this SWC approximation such as the susceptibility

$$\chi_{zz}^{(\text{SWC})}(q) = \frac{1}{\pi^2} \left| \frac{q}{\sin q} \right| \quad (5)$$

and the static correlation function

$$C_{zz}^{(\text{SWC})}(q) = \frac{1}{\pi} \ln \left(\frac{1 + |\sin(q/2)|}{\cos(q/2)} \right). \quad (6)$$

The latter yields the asymptotic behaviour $C_{zz}^{(\text{SWC})}(R) \propto (-1)^R/R$ in real space. These results are quite distinct from the predictions of classical spin-wave theory. Moreover, the spectral weight function (4) showing increasing asymmetry as $q \rightarrow \pi$ is in good agreement with recent neutron scattering data on CPC [1].

The case $h \neq 0$ has already been sketched qualitatively in [2] and [3]. Finite-chain calculations show that two different classes of states give predominant contributions to G_{zz} . Fig. 1 shows the result for a 10-spin ring. For a given field h the ground state has total spin S^T , corresponding to a magnetisation $\sigma = S^T/N$. One of these classes contains excitations with the same total spin S^T and the other states with total spin $S^T + 1$. We have identified each one of these states with an eigenstate in the Bethe formalism and showed that, in the thermodynamic limit, each class forms a continuum of excitations. The boundaries of these continua, which depend on the solution of an integral equation, can be determined exactly for $h = 0$ [3, 5] and $h = 2$, the critical field. For intermediate fields Ishimura and Shiba [6] obtained a numerical result for the lowest branch. In order to obtain analytical - albeit approximate - expressions we make an ansatz for the solution of the above-mentioned integral equation which consists of a superposition of the known solutions for $h = 0$ and $h = 2$ with weights A and $1 - A$, respectively. This yields lower and upper boundaries for the higher continuum ($q_s \leq q \leq \pi$):

$$E_{\text{HL}}(q) = 2D \sin \frac{q}{2} \cos \left(\frac{q}{2} - \frac{q_s}{2} \right), \quad E_{\text{HU}}(q) = 2D \sin \frac{q}{2}, \quad (7)$$

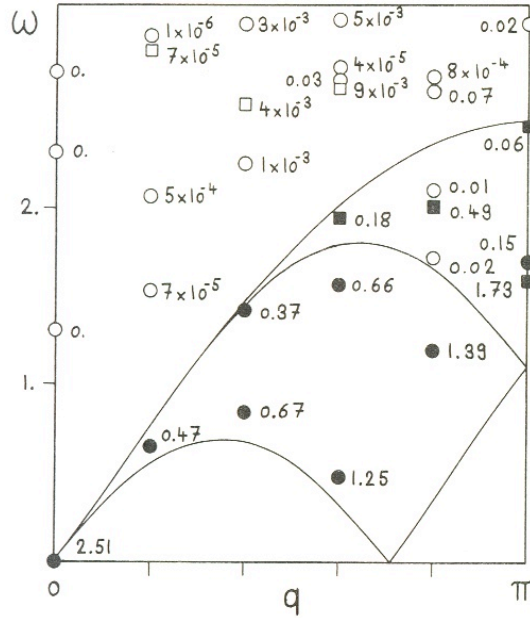


Figure 1. This figure represents the contributions to $G_{zz}(q, \omega)$ according to eq. (3) for a cyclic chain of $N = 10$ spins in a magnetic field $h = 1.12$. The circles (squares) denote energy and wave number of the excitations with total spin $S^T = 2$, ($S^T = 3$). The numbers represent the corresponding spectral weight $2\pi |\langle 0 | S_z(q) | \lambda \rangle|^2$. The ground-state at $q = 0$ and $\omega = 0$ also has $S^T = 2$. The two classes of excitations described in the text, which have dominating spectral weight, are characterized by full symbols. In the thermodynamic limit they form two continua of excitations, the boundaries of which (full lines) are given approximately by eqs. (7) and (8). Higher lying excitations not contained in the figure have negligible spectral weight.

and the lower continuum ($0 \leq q \leq \pi$):

$$E_{LL}(q) = 2D \left| \sin \frac{q}{2} \cos \left(\frac{q}{2} + \frac{q_s}{2} \right) \right|, \quad E_{LU}(q) = E_{HL}(q). \quad (8)$$

Here $q_s = 2\pi\sigma$ and $D = A(\pi/2 - 1) + 1$. There is an exact relation between the field h and the excitation energy E_{HL} at the zone boundary: $E_{HL}(\pi) = 2D \sin(\pi\sigma) = h$. This determines the parameter D as a function of σ and h . Conversely, we obtain for the magnetisation $\sigma = \pi^{-1} \arcsin(h/2D)$. For zero field, $D = \pi/2$, reproducing the exact zero-field susceptibility $\chi_{zz} = \pi^{-2}$. At the critical field, $D = 1$ and $\chi_{zz} \propto (h_c - h)^{-1/2}$. The simplest interpolation for intermediate fields is certainly $A = 1 - h/2$. This leads to the explicit form ($0 \leq h \leq 2$):

$$\sigma = \frac{1}{\pi} \arcsin \left(\frac{h}{(1 - h/2)(\pi - 2) + 2} \right) \quad (9)$$

for the magnetisation, which is in excellent agreement with the exact result obtained numerically by Griffiths [7].

The numerical values of the matrix elements for the finite chains suggest that, in the thermodynamic limit, $G_{zz}(q, \omega)$ diverges at the lower boundaries of both continua. Analogous calculations show that G_{xx} is also dominated by several continua of excitations. However, the lowest branch is inverted with respect to the axis $q = \pi/2$. Inelastic neutron spectra are therefore expected to be more complex than for $h = 0$, having at least two peaks for wave-vectors $2\pi\sigma < q < \pi$. This seems to be borne out by the recent experiments on CPC [1] in a magnetic field.

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