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Temperature and Field Dependence of Autocorrelation Functions for the One-Dimensional Heisenberg Antiferromagnet

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We present analytical and numerical results for the low frequency autocorrelation function of the l-d $s = \frac{1}{2}$ Heisenberg antiferromagnet at low temperature and various fields. Our results are in good agreement with NMR data.

The low temperature magnetic properties of the copper salts $\mathrm{CuSO_4 \cdot 5H_2O}$, $\mathrm{CuSeO_4 \cdot 5H_2O}$, $\mathrm{CuBeF_4 \cdot 5H_2O}$ can be described by treating the crystal as a system of loosely coupled $s = \frac{1}{2}$ antiferromagnetic chains [1] with Hamiltonian

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

Recently [l] the dynamics of the Cu spins belonging to such chains has been investigated by NMR, performed on the protons of the H_2O-molecules. Basically the inverse "spin-lattice" relaxation time T_1 characterizing the influence of the Cu spins on the proton moments (due to dipolar interactions) is determined by the dynamical autocorrelation functions of the chain spins [1]:

$$\phi_{\alpha\alpha}(\omega) \equiv \int dt\, e^{i\omega t} \langle S_\alpha(t) S_\alpha(0) \rangle, \quad 1/T_1 = A_z \phi_{zz}(\omega_\mathrm{N}) + A_x \phi_{xx}(\omega_\mathrm{N}). \tag{2}$$

A_x and A_z depend on geometry. The nuclear Larmor frequency ω_N is small compared to the exchange constant (our unit of energy) and will therefore be replaced by zero.

In order to calculate T_1^{-1} we need the functions $\phi_{zz}(0)$ and $\phi_{xx}(0)$ for the Hamiltonian (1) at various temperatures and fields. $\phi_{zz}(0)$ was calculated [2] assuming the low-temperature dynamics to be governed by a single branch of non-interacting, sharp spin-waves. This assumption leads directly to a divergence of $\phi_{zz}(0)$ for $T = 0$. On the other hand, experiments on $s = \frac{1}{2}$ systems [1, 2] point to a finite limit of $\phi_{zz}(0)$. Recently the field dependence of T_1 for various T has been measured [3] up to fields above the critical value $h_\mathrm{c} = 2$.

In a recent paper [4] we presented an approximate analytic expression for the dynamic spin correlation functions in (q, ω)-space at $T = 0$ and $h = 0$, taking into account excitations from the (singlet) ground state to the spin-wave continuum of triplet states:

$$G_{xx}(q, \omega) = 2\big[\omega^2 - E_\mathrm{L}^2(q)\big]^{-1/2} \Theta\big(\omega - E_\mathrm{L}(q)\big) \Theta\big(E_\mathrm{U}(q) - \omega\big). \tag{3}$$

Here $E_\mathrm{L}(q) = (\pi/2)|\sin q|$ and $E_\mathrm{U}(q) = \pi|\sin(q/2)|$. Our autocorrelation function $\phi_{xx}(\omega)$ is immediately found by integration over q. It shows a logarithmic divergence at $\omega = \pi/2$, and the zero frequency limit is

$$\phi_{xx}(\omega) = 2/\pi + \mathrm{O}(\omega). \tag{4}$$

Obviously, for $h = 0$,

$$\phi_{zz}(\omega) = \phi_{xx}(\omega).$$

For fields $h \geq h_c$ Bethe's formalism yields the exact result (for $T = 0$):

$$\phi_{xx}(\omega) = \frac{1}{2}\big[1 - (1 + h - h_c - \omega)^2\big]^{-1/2}\Theta\big(\omega - (h - h_c)\big)\Theta\big(2 + h - h_c - \omega\big). \tag{5}$$

At the critical field $\phi_{xx}(0)$ diverges, whereas it vanishes for $h > h_c$. For $0 < h < h_c$ finite-chain calculations suggest that the dominant contribution to $\phi_{xx}(0)$ again comes from excitations near $q = \pi$, as for $h = 0$ and $h = h_c$. Bethe's formalism allows for an approximate calculation of the lower boundary of that spin-wave continuum which contributes to ϕ_{xx} [5]:

$$E_L(q) = 2D|\cos(q/2)\sin(q/2 - \pi\sigma)|, \tag{6}$$

where $D = (1 - h/2)(\pi/2 - 1) + 1$ and σ is the magnetization, given by $\sigma = \pi^{-1}\arcsin(h/2D)$. Assuming that the spectral weight of $G_{xx}(q, \omega)$ above $E_L(q)$ still has a square root behaviour as in eq. (3) the q-integration yields

$$\phi_{xx}(0) = 2\big(4D^2 - h^2\big)^{-1/2}. \tag{7}$$

At zero field $\phi_{xx}(0) = 2/\pi$ and at the critical field $\phi_{xx}(0)$ diverges. Essentially the same behaviour of $\phi_{xx}(0)$ as in eq. (7), has been found by Groen et al. [6] using a completely different approach.

Since an analytical treatment for finite temperatures seems to be out of reach for the time being, we also performed numerical calculations for finite chains. In fig. 1 the field dependence of $\phi_{xx}(0) = 2/\pi$ for a cyclic chain of 8 spins at $T = 0.17$ (corresponding to 0.5 K for $CuSO_4$) is compared with very recent experimental values for T_1^{-1} obtained by Groen [7] and with eq. (7). [The geometry of these experiments was chosen such that the constant A_z in our eq. (2) was zero.] Our results for higher T are also in good agreement with the experimental data of ref. [3]. Details will be published elsewhere.

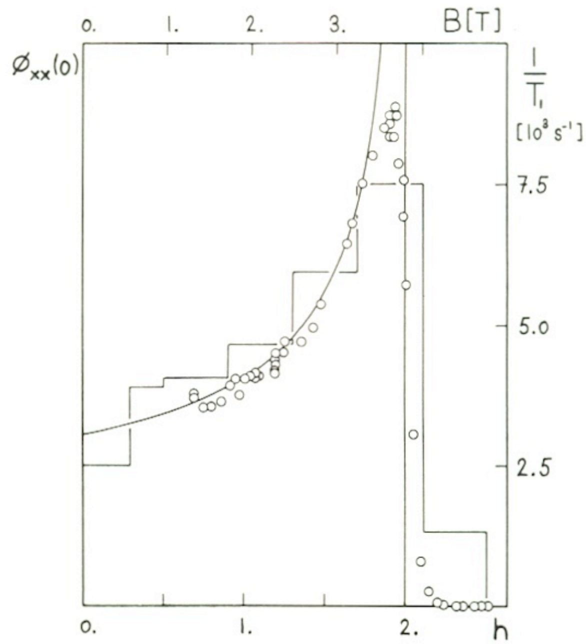

Figure 1. This figure shows the field dependence of the transverse autocorrelation function $\phi_{xx}(\omega = 0)$. The histogram represents the result for a cyclic chain containing 8 spins at a reduced temperature $T = 0.17$ and the continuous curve the result (7) of our spin-wave continuum approach at $T = 0$. The circles denote experimental values of the inverse relaxation time T_1^{-1} obtained by Groen (7) on $CuSO_4$ for a geometry with $T_1^{-1} \propto \phi_{xx}(0)$. The magnetic field B is given in tesla. Both theoretical curves are scaled independently in order to compare them directly with the data points.

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