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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 1-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 CuSO$_4$·5H$_2$O, CuSeO$_4$·5H$_2$O, CuBeF$_4$·5H$_2$O can be described by treating the crystal as a system of loosely coupled $s = \frac{1}{2}$ antiferromagnetic chains [1] with Hamiltonian

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

(1)

Recently [1] the dynamics of the Cu spins belonging to such chains has been investigated by NMR, performed on the protons of the H$_2$O-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]:

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

(2)

$A_z$ and $A_x$ depend on geometry. The nuclear Larmor frequency $\omega_N$ 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 $h_c = 2$.

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

$$G_{xx}(q, \omega) = 2 \left[ \omega^2 - E^2_L(q) \right]^{-1/2} \Theta(\omega - E_L(q)) \Theta(E_U(q) - \omega).$$

(3)

Here $E_L(q) = (\pi/2) |\sin q|$ and $E_U(q) = \pi |\sin(q/2)|$. 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

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

(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 \( T = 0 \)):

\[
\phi_{xx}(\omega) = \frac{1}{2} \left[ 1 - (1 + h - h_c - \omega)^2 \right]^{-1/2} \Theta(\omega - (h - h_c)) \Theta(2 + h - h_c - \omega).
\]

(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 \( \phi_{xx} [5] \):

\[
E_L(q) = 2D[\cos(q/2) \sin(q/2 - \pi \sigma)],
\]

(6)

where \( D = (1 - h/2)(\pi/2 - 1) + 1 \) and \( \sigma \) 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

\[
\phi_{xx}(0) = 2 \left( 4D^2 - h^2 \right)^{-1/2}.
\]

(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 \( T^{-1} \) 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 \( T^{-1} \) obtained by Groen (7) on CuSO\(_4\) for a geometry with \( T^{-1} \propto \phi_{xx}(0) \). 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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References

5. G. Müller, H. Beck and J. C. Bonner, same issue.
7. J. P. Groen, private communication