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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 1d \(s = \frac{1}{2}\) 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 \(\text{CuSO}_4 \cdot 5\text{H}_2\text{O}, \text{CuSeO}_4 \cdot 5\text{H}_2\text{O}, \text{CuBeF}_4 \cdot 5\text{H}_2\text{O}\) 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 [1] the dynamics of the Cu spins belonging to such chains has been investigated by NMR, performed on the protons of the \(\text{H}_2\text{O}\)-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]:

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

\(A_z\) 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:

\[
G_{xx}(q, \omega) = 2 \left[ \omega^2 - E_L^2(q) \right]^{-1/2} \Theta(\omega - E_L(q)) \Theta(E_U(q) - \omega). \tag{3}
\]

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

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

Obviously, for \(h = 0\),

\[
\phi_{zz}(\omega) = \phi_{xx}(\omega).
\]
For fields $h \geq h_c$ Bethe’s formalism yields the exact result (for $T = 0$):

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

$$E_L(q) = 2D \cos(q/2) \sin(q/2 - \pi \sigma),$$  \hspace{1cm} (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

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