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Dynamical Correlation Functions for Linear Spin Chains

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Dynamical spin correlation functions are calculated numerically for cyclic linear Heisenberg chains containing up to 10 spins with $S = \frac{1}{2}$ and $S = 1$. We consider ferro- and antiferromagnets including single-site and exchange anisotropies. The results agree well with the neutron scattering cross sections on quasi one-dimensional systems.

The properties of quasi one-dimensional magnetic materials have recently been reviewed [1]. Some prominent examples are: TMMC ($S = \frac{5}{2}$ Heisenberg antiferromagnet (HB AF)), CPC ($S = \frac{1}{2}$ HB AF), $CsNiF_3$ ($S = 1$ planar HB Ferromagnet (FM)). The dynamics of such weakly coupled spin chains is investigated by neutron scattering. The experimental results show rather well defined spin-wave peaks at low temperatures. Unfortunately, a rigorous theoretical treatment of the dynamics of HB chains is impossible.

Thus besides various analytical approaches (see [1]), some authors have evaluated the dynamical spin correlation functions numerically by diagonalizing the Hamiltonian of finite chains. Richards and Carboni [2] demonstrated the existence of spin-wave peaks at low T for isotropic HB AF $S = \frac{1}{2}$ chains. The purpose of this work is to extend these calculations to various anisotropic systems and to $S > \frac{1}{2}$. We treat the Hamiltonian

$$H = \pm J \sum_{l=1}^{N} \Big\{ \alpha S_z(l) S_z(l+1) + \beta \big[S_x(l) S_x(l+1) + S_y(l) S_y(l+1) \big] \Big\} + \gamma \sum_{l=1}^{N} S_z^2(l) \qquad (1)$$

for a chain of N sites with periodic boundary conditions. The eigenfunctions of (1) can be classified by S_z^T (z-component of total spin) and a k-vector ($k = n2\pi/N, n = 0, \dots, N-1$). Using the eigenvalues E_λ and eigenvectors $|\lambda\rangle$ we evaluate

$$\begin{aligned} G_{\alpha\alpha}(q,\omega) &= N^{-1} \sum_{ll'} \mathrm{e}^{\mathrm{i}q(l-l')} \int \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\omega t} \langle S_\alpha(l,t) S_\alpha(l',0) \rangle \\ &= \frac{2\pi}{Z} \sum_{\lambda\lambda'} \mathrm{e}^{-\beta E_\lambda} \delta(\omega + E_\lambda - E_{\lambda'}) |\langle \lambda | S_\alpha(q) | \lambda' \rangle|^2. \end{aligned} \qquad (2)$$

For finite systems these functions are best represented, for fixed q, as histograms in frequency space. In the following we describe our main results for various cases:

(i) *Isotropic HB AF.* In agreement with [2] we obtain Gaussian line shapes (spin diffusion) for $T \to \infty$ and spin-wave peaks for low T. These peaks are predominantly produced by matrix elements between the ground state, which has $K_0 = 0$ or $K_0 = \pi$ depending on N, and the lowest eigenstates with wave vector $q + k_0$. The latter were determined exactly by Des Cloiseaux and Pearson (DP), see [1], for infinite chains. However, even at $T = 0$, states with higher energies also contribute in agreement with theoretical considerations by Hohenberg and Brinkman [3].

(ii) *Isotropic HB FM.* Here, at $T = 0$, the spin-wave peaks are sharp. All nonzero matrix elements, i.e. those between each of the degenerate ground states and the corresponding spin-wave states, contribute to $G_{\alpha\alpha}$ at the same frequency. For finite, but low, T additional contributions arise from spin-wave bound states, which, at least for small q, again contribute at frequencies close to the $T = 0$ spin-wave frequency. Therefore, for low T, the peak is narrower for a FM than for an AF chain.

(iii) *HB FM with anisotropic exchange* ($\alpha < \beta, \gamma = 0$). For $\alpha \neq \beta$ the lowering of the symmetry partially lifts the degeneracies of the isotropic HB chain: the energies depend on $|S_z^T|$, and G_{xx} and G_{zz} are no more identical. Due to selection rules, only states with the same S_z^T are connected for G_{zz}. However, these states are all affected in a similar way by the anisotropy. The matrix elements for G_{xx} are those with $\Delta S_z^T = \pm 1$, i.e. between states that are shifted differently by anisotropy. Thus the peak of G_{zz} is narrower than the one of G_{xx} for $\alpha < \beta$. In the extreme case $\alpha = 0$ (XY-chain) G_{zz} has one sharp peak at $T = 0$ and the smallest q ($= 2\pi/N$), whereas for larger wave-vectors several peaks appear. G_{xx} shows a broad 'background' accompanying the main peak, which is due to the one-fermion states in the treatment of Lieb, Schultz and Mattis (LSM), see [1].

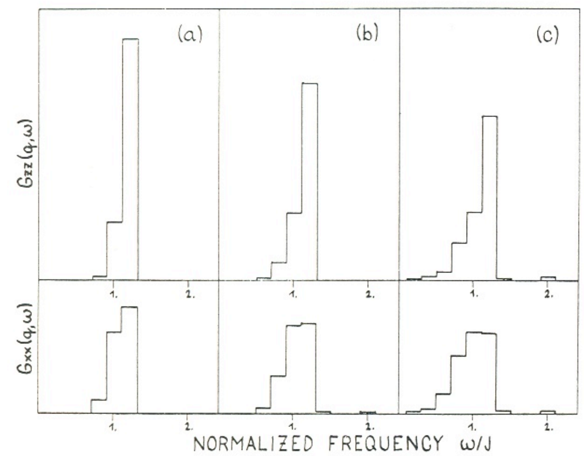

Figure 1. In-plane (G_{xx}) and out-of-plane (G_{zz}) correlation function at $q = \pi/3$ for the planar HB FM $S = 1$ chain of 6 particles. The value $\gamma = 0.212J$ for the anisotropy is appropriate for $CsNiF_3$, [4] and q is close to $q_z = 0.35\pi$ used in neutron scattering [4]. The three temperatures correspond to those of ref. 4: (a) $T = 0.208J$, (b) $T = 0.343J$, (c) $T = 0.5J$.

(iv) *Planar HB FM* ($\alpha = \beta, \gamma > 0$. This model is appropriate for $CsNiF_3$ [I, 4]. Histograms of G_{xx} and G_{zz} are shown in fig. 1 for $q = \pi/3$ and various T. Our results are in good qualitative agreement with neutron scattering data. The main peak of G_{zz} is narrow and decreases rather rapidly with rising T, without shifting appreciably in energy. In contrast G_{xx} shows a broader shape. Its width and intensity both increase with growing T. The energies of the lowest states connected with the ground state by $S_x(q)$ and $S_z(q)$ follow closely the dispersion relation

$$\omega^2(q) = 4J^2S^2\big\{(1 - \cos q)(1 - \cos q + \gamma/J)\big\} \tag{3}$$

given by Villain [1, 4]. The local anisotropy ($\gamma > 0$) splits the degenerate eigenvalues of the isotropic system in a way similar to the case $\alpha \neq \beta$ described before. Thus the rather distinct behaviour of G_{zz} and G_{xx} is again due to the shifts produced by the (single-site) anisotropy and the S_z^T selection rules. More details will be published elsewhere. We have used a modified cmpj.sty style file.

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