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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

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

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

\[ G_{\alpha\alpha}(q,\omega) = N^{-1} \sum_{l,l'} \text{e}^{iql-l'} \int dt \text{e}^{i\omega t} \langle S_{\alpha}(l,t)S_{\alpha}(l',0) \rangle \]

\[ = \frac{2\pi}{Z} \sum_{\lambda\lambda'} e^{-\beta E_{\lambda}} \delta(\omega + E_{\lambda} - E_{\lambda'}) \langle \lambda | S_{\alpha}(q) | \lambda' \rangle^2. \]  

(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 \(|S_T^z|\), and \(G_{xx}\) and \(G_{zz}\) are no more identical. Due to selection rules, only states with the same \(S_T^z\) 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 \(\Delta S_T^z = \pm 1\), 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](image-url) **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

\[
\omega^2(q) = 4J^2S^2\{(1 - \cos q)(1 - \cos q + \gamma/J)\}
\]

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 \(S_T^z\) selection rules. More details will be published elsewhere. We have used a modified cmpj.sty style file.

**References**