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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

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

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

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

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

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 $T \rightarrow \infty$ 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 (α < β, γ = 0). For α ≠ β the lowering of the symmetry partially lifts the degeneracies of the isotropic HB chain: the energies depend on |STz|, and Gxx and Gzz are no more identical. Due to selection rules, only states with the same S′Tz are connected for Gzz. However, these states are all affected in a similar way by the anisotropy. The matrix elements for Gxx are those with ∆STz = ±1, i.e. between states that are shifted differently by anisotropy. Thus the peak of Gzz is narrower than the one of Gxx for α < β. In the extreme case α = 0 (XY-chain) Gzz has one sharp peak at T = 0 and the smallest q (= 2π/N), whereas for larger wave-vectors several peaks appear. Gxx 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].

(iv) Planar HB FM (α = β, γ > 0). This model is appropriate for CsNiF3 [I, 4]. Histograms of Gxx and Gzz are shown in fig. 1 for q = π/3 and various T. Our results are in good qualitative agreement with neutron scattering data. The main peak of Gzz is narrow and decreases rather rapidly with rising T, without shifting appreciably in energy. In contrast Gxx 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 Sx(q) and Sz(q) follow closely the dispersion relation

\[ \omega^2(q) = 4J^2S^2\left\{(1 - \cos q)(1 - \cos q + \gamma/J)\right\} \] (3)

given by Villain [1, 4]. The local anisotropy (γ > 0) splits the degenerate eigenvalues of the isotropic system in a way similar to the case α ≠ β described before. Thus the rather distinct behaviour of Gzz and Gxx is again due to the shifts produced by the (single-site) anisotropy and the S′Tz selection rules. More details will be published elsewhere. We have used a modified cmpj.sty style file.

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