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LETTER TO THE EDITOR

Dynamical structure factor for Haldane-gap antiferromagnets

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Abstract. The dynamical properties of a spin-1 chain with single-ion easy-plane anisotropy are studied by a Green's function technique. The longitudinal and transverse dynamical structure factors (DSFs) have been obtained from the imaginary part of the Green's functions. The static DSFs as a function of the momentum are numerically calculated.

Haldane [1] first argued that integer-spin S antiferromagnetic (AFM) Heisenberg chains have a singlet ground state which has a gap to a triplet excited state. This has been well confirmed both experimentally and theoretically for the $S = 1$ system. Recently, detailed inelastic neutron-scattering experiments [2] were carried out on $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ (NENP), measuring the dynamical structure factor (DSF) $S(k, \omega)$ for $k \geqslant 0.3\pi$. The DSF crosses over from one-magnon to two-magnon behaviour as k is swept across the Brillouin zone. Golinelli *et al* [3] have studied the dynamic spin correlation function of a spin-1 AFM chain with easy-plane single-ion anisotropy using the exact diagonalization by the Lanczos method for chain lengths of up to $N = 16$ spins. Takahashi [4] used the diagonalization method and calculated not only the first excited state but also higher excited states and their contribution to the DSF. Sorensen and Affleck [5] presented results on the equal time structure function $S(k)$ using the density-matrix renormalization-group method with chain length $L = 100$. They found that at $k \approx \pi$ a single-magnon process dominates, whereas at $k \approx 0$ a two-magnon process dominates.

In our previous paper [6] we have calculated the excitation spectrum of an infinite one-dimensional spin-1 AFM Heisenberg chain with both exchange anisotropy and single-ion anisotropy by a Green's function technique. The aim of the present paper is to calculate the DSF from the imaginary part of the Green's function for Haldane-gap AFMs.

NENP, which is one of the most promising candidates for a Haldane-gap system, is not isotropic. The largest of the anisotropies is the single-ion anisotropy D. The Hamiltonian which describes NENP well is given by

$$H = \sum_i \left[J \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D(S_i^z)^2 \right] \tag{1}$$

with $D/J = 0.2$ and $J = 3.8$ meV [2]. For the approximate calculation of the Green's function $G_k(t) = -i\Theta(t) = \langle [B_k(t), B_k^+] \rangle$ with the operators B_k, B_k^+ we use a method proposed by Tserkovnikov [7] which is appropriate for spin problems. After a formal integration of the equation of motion for the Green's function one obtains

$$G_k(t) = -i\Theta(t) \langle [B_k, B_k^+] \rangle \exp(-iE_k(t)t) \tag{2}$$

where

$$E_k(t) = \epsilon_k - \frac{i}{t} \int_0^t dt' t' \left\{ \frac{\langle [j_k(t), j_k^+(t')] \rangle}{\langle [B_k(t), B_k^+(t')] \rangle} - \frac{\langle [j_k(t), B_k^+(t')] \rangle \langle [B_k(t), j_k^+(t')] \rangle}{\langle [B_k(t), B_k^+(t')] \rangle^2} \right\} \tag{3}$$

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with the notation $j_k = [B_k, H_{int}]$. The time-independent term

$$\epsilon_k = \frac{\langle [[B_k, H], B_k^+] \rangle}{\langle [B_k, B_k^+] \rangle} \tag{4}$$

gives the excitation spectrum in the generalized Hartree–Fock approximation. The time-dependent term includes the damping effects. Calculations yield the following expressions for the Green's functions for the transverse and longitudinal excitations [6]:

$$G^{xx}(k, \omega) = \frac{4\langle S_0^- S_0^+ \rangle \epsilon_{11}}{\omega^2 - \epsilon_k^2 + 2\mathrm{i}\omega\gamma_k^{11}} \tag{5}$$

and

$$G^{zz}(k, \omega) = \frac{2\langle S_0^z S_0^z \rangle}{\omega - \epsilon^z(k) + \mathrm{i}\gamma_k^{zz}} \tag{6}$$

with

$$\epsilon(k) = \frac{1}{2}\left[\epsilon_{11} + \epsilon_{22} \pm \sqrt{(\epsilon_{11} - \epsilon_{22})^2}\right] \tag{7}$$

$$\begin{aligned}\epsilon_{11}(k) = \frac{1}{2\langle S_0^- S_0^+ \rangle}\Big[& J\big(\langle S_0^+ S_1^- \rangle \cos k - 2\langle S_0^z S_1^z \rangle - 2\langle S_{-1}^z S_0^z \rangle + \langle S_{-1}^- S_0^+ \rangle \cos 2k \\ & - \langle S_{-1}^+ S_0^- \rangle - 2\langle S_{-1}^z S_0^- \rangle \cos 2k - 2\langle S_0^z S_1^z \rangle \cos k + \langle S_0^- S_1^+ \rangle\big) \\ & + D\left(\langle S_0^+ S_0^- \rangle - 4\langle S_0^z S_0^z \rangle + \langle S_0^- S_0^+ \rangle\right)\Big]\end{aligned} \tag{8}$$

$$\begin{aligned}\epsilon_{22}(k) = \frac{1}{2\langle S_0^+ S_0^- \rangle}\Big[& J\big(\langle S_0^- S_1^+ \rangle \cos k - 2\langle S_0^z S_1^z \rangle - 2\langle S_{-1}^z S_0^z \rangle + \langle S_{-1}^+ S_0^- \rangle \cos 2k \\ & - \langle S_0^+ S_1^- \rangle - 2\langle S_0^z S_1^z \rangle \cos k + \langle S_{-1}^- S_0^+ \rangle - 2\langle S_{-1}^z S_0^z \rangle \cos 2k\big) \\ & + D\left(\langle S_0^- S_0^+ \rangle - 4\langle S_0^z S_0^z \rangle + \langle S_0^+ S_0^- \rangle\right)\Big] = -\epsilon_{11}(k)\end{aligned} \tag{9}$$

$$\begin{aligned}\epsilon^z(k) = \frac{1}{2\langle S_0^z S_0^z \rangle}\Big[& \frac{J}{2}\big(\langle S_0^+ S_1^- \rangle \cos k - \langle S_0^+ S_1^- \rangle - \langle S_{-1}^+ S_0^- \rangle + \langle S_{-1}^+ S_0^- \rangle \cos 2k \\ & + \langle S_0^- S_1^+ \rangle \cos k - \langle S_0^- S_1^+ \rangle - \langle S_{-1}^- S_0^+ \rangle + \langle S_{-1}^- S_0^+ \rangle \cos 2k\big) \\ & + J\big(\langle S_0^+ S_1^z S_1^- \rangle \cos k - \langle S_0^+ S_0^z S_1^- \rangle - \langle S_{-1}^+ S_0^z S_0^- \rangle + \langle S_{-1}^+ S_{-1}^z S_0^- \rangle \cos 2k \\ & - \langle S_0^- S_1^z S_1^+ \rangle \cos k + \langle S_0^- S_0^z S_1^+ \rangle + \langle S_{-1}^- S_0^z S_0^+ \rangle - \langle S_{-1}^- S_{-1}^z S_0^+ \rangle \cos 2k\big)\Big].\end{aligned} \tag{10}$$

The correlation functions are calculated from the Green's functions using the spectral theorem [6]. For the transverse and longitudinal damping we obtain, respectively:

$$\begin{aligned}\gamma^{11}(k) = \frac{\pi J^2}{\langle S_0^- S_0^+ \rangle}\Big[& \left(\langle S_0^z S_{-1}^z S_0^z \rangle - \langle S_{-1}^+ S_0^z S_{-1}^- \rangle \cos 2k\right) \delta\left(\epsilon_{2k} - \epsilon_0^z - \epsilon_0\right) \\ & + \left(\langle S_0^z S_1^z S_0^z \rangle - \langle S_1^- S_0^z S_1^+ \rangle \cos k\right) \delta\left(\epsilon_k - \epsilon_0^z - \epsilon_0\right)\Big]\end{aligned} \tag{11}$$

$$\begin{aligned}\gamma^{zz}(k) = \frac{\pi J^2}{4\langle S_0^z S_0^z \rangle}\Big[& \left(\langle S_1^+ S_0^z S_1^- \rangle \cos k - \langle S_0^+ S_1^z S_0^- \rangle + \langle S_1^- S_0^z S_1^+ \rangle \cos k - \langle S_0^- S_1^z S_0^+ \rangle\right) \\ & \delta\left(\epsilon_0 - \epsilon_k + \epsilon_0^z\right) + \left(\langle S_{-1}^+ S_0^z S_{-1}^- \rangle - \langle S_0^+ S_{-1}^z S_0^- \rangle \cos 2k + \langle S_{-1}^- S_0^z S_{-1}^+ \rangle\right. \\ & \left. - \langle S_0^- S_{-1}^z S_0^+ \rangle \cos 2k\right)\delta\left(\epsilon_0 - \epsilon_{2k} + \epsilon_0^z\right)\Big]\end{aligned} \tag{12}$$

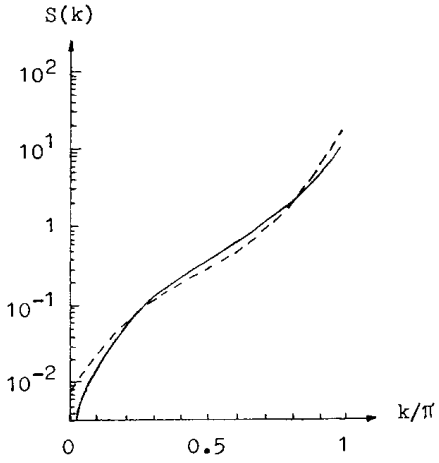

Figure 1. Structure factor $S^{zz}(k)$ (full curve) and $S^{xx}(k)$ (dashed curve) of the $S = 1$ anisotropic infinite Heisenberg chain with $D/J = 0.2$ and $J = 3.8$ meV.

with the positive square root of $\epsilon(k)$ from equation (7). The single-ion anisotropy D gives contribution to the damping through the higher correlation functions $\langle S_0^+ S_1^z S_0^- \rangle$ etc. [6]. From the imaginary part of $G^{xx}(k, \omega)$ and $G^{zz}(k, \omega)$ we obtain the transverse and longitudinal DSFs $S(k, \omega)$:

$$S(k, \omega) = -\frac{1}{\pi} \mathrm{Im} G(k, \omega). \tag{13}$$

In the isotropic $D = 0$ case the ground state is a singlet and thus $S(k = 0, \omega) = 0$. The vanishing with k will occur quadratically. In the presence of easy-plane anisotropy the ground state is invariant only under z rotations and thus $S^{zz}(k = 0, \omega) = 0$, while $S^{xx} = S^{yy}$ will be non-zero at $k = 0$. With in-plane anisotropy even $S^{zz}(k = 0, \omega)$ will be non-zero.

The static DSFs $S(k)$ obtained by integration over frequency are numerically calculated in the -1 state and shown in figure 1. Near $k = 0$, $S^{zz}(k)$ approaches zero. The transverse structure factor $S^{xx}(k)$ can take on a non-zero value at $k = 0$ because the rotational symmetry around the x and y axis is broken. S^{xx} and S^{zz} cross around $k/\pi = 0.1$ and 0.8. In the range $0.1 < k/\pi < 0.8$, S^{zz} is larger than S^{xx}. The results are in good agreement with the theoretical results of Sorensen and Affleck [5], and with the experimental data for NENP of Ma *et al* [2]. We believe that the Green's function method of Tserkovnikov [7] used here is still a very useful technique for investigating the dynamical properties of the Heisenberg chains.

References

[1] Haldane D M 1983 *Phys. Rev. Lett.* **50** 1153
Haldane D M 1983 *Phys. Lett.* **93** A 464
[2] Ma S, Broholm C, Reich D H, Sternlieb B J and Erwin R W 1992 *Phys. Rev. Lett.* **69** 3571
[3] Golinelli O, Jolicoeur Th and Lacaze R 1993 *J. Phys.: Condens. Matter* **5** 1399
[4] Takahashi M 1994 *Phys. Rev.* B **50** 3045
[5] Sorensen E S and Affleck I 1994 *Phys. Rev.* B **49** 13235
[6] Wesselinowa J M 1998 *Phys. Status Solidi* b **206** 805
[7] Tserkovnikov Yu A 1971 *Teor. Math. Fiz.* **7** 250