Calculation of the out-of-plane dynamical correlation for $CsNiF_3$

S. A. Leonel
Departamento de Fisica, Universidade Federal de Juiz de Fora, Juiz de Fora, Minas Gerais, Brazil

A. S. T. Pires
Departamento de Fisica, Universidade Federal de Minas Gerais, CP 702, Belo Horizonte, 30161970 Minas Gerais, Brazil

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We calculate the out-of-plane dynamical spin correlation function for the one-dimensional easy-plane ferromagnet $CsNiF_3$ at low temperatures using a diagrammatic expansion for the temperature-dependent Green function. We compare our theoretical calculation for the spin wave linewidth with experimental data of Kakurai, Steiner, and Dorner. [S0163-1829(96)02842-1]

In the past years the spin dynamics of one-dimensional (1D) magnetic systems have been studied extensively both theoretically and experimentally.[1–3] The Hamiltonian

$$H=-2J\sum_i \vec{S}_i\cdot\vec{S}_{i+1}+A\sum_i (S_i^z)^2, \tag{1}$$

with $S=1$, has been found to describe the easy-plane ferromagnet $CsNiF_3$ quite well. The values of the parameters for this compound were obtained by Steiner, Dorner, and Villain[4] from the low temperature classical spin wave dispersion relation measured in neutron scattering experiments.[5] This procedure yields $J=11.5$ K and $A=4.5$ K. A quantum renormalization of the Hamiltonian[6] (1) however reduces A to $A\ (1-1/(2S))$ which yields $A=9.0$ K. We have found that using the value $A=9.0$ K (bare parameter) in our theoretical calculation we could fit the experimental data for the spin wave peak position quite well. In zero field, the most important excitation in this system is the spin-wave-like propagating modes for wave vectors q larger than the inverse correlation length $k(T)$. Villain[7] using a self-consistent harmonic approximation predicted the existence of two characteristic linewidths, due to in-plane (IP) and out-of-plane (OP) spin fluctuations. The IP component of the dynamic structure factor $S^{\alpha\alpha}(q,\omega)(\alpha=x,y)$ has been quite well studied showing a well behaved structure.[8] However the linewidth of the OP component $S^{zz}(q,\omega)$ displays an anomalous wave vector dependence due to a singularity in the three spin wave density of states. This anomalous behavior was predicted by Reiter[9] using a classical zero-temperature spin wave theory, and observed in $CsNiF_3$ by Kakurai, Steiner, and Dorner[8] by means of inelastic polarized neutron scattering.

In this Brief Report we will calculate the in-plane dynamic structure factor for the quantum Hamiltonian (1). We will take the classical easy-plane ferromagnetic state as the zeroth approximation, and expand in powers of the amplitude of the out-of-plane fluctuations $\langle (S_n^z)^2\rangle/[S(S+1)]$, and in-plane fluctuations $\langle(\phi_n-\phi_{n+1})^2\rangle$. In a diagrammatic expansion of the perturbation series for semiclassical spin the leading term is the classical system, one-loop graphs are of order $\hbar$, two-loop graphs of order $\hbar^2$, and so on.[10] More accurately, the graphs are of order $1/S$, $1/S^2$, etc., and for a semiclassical system $\hbar S$ is of order unity. We will carry out the expansion to the two-loop level, which involves computation of 46 different diagrams. The multiplicity of diagrams and their greater complexity make it impractical to go beyond two loops.

We start by introducing the Villian's representation[7]

$$S_n^+=e^{i\phi_n}[S(S+1)-S_n^z(S_n^z+1)]^{1/2},$$

$$S_n^-=[S(S+1)-S_n^z(S_n^z+1)]^{1/2}e^{i\phi_n}, \tag{2}$$

where ϕ is the angular variable in the xy plane canonically conjugated to S_n^z. Substitution of (2) into the Hamiltonian (1), expanding to second order in $S_n^z/\sqrt{S(S+1)}$ and $(\phi_n-\phi_{n+1})$, and Fourier transforming gives

$$H=E_0+H_2+H_4+\cdots, \tag{3}$$

where $E_0=-2JNS(S+1)$ is the energy of the classical ground state, H_2 is the harmonic Hamiltonian given by

$$H_2=2JS(S+1)\sum_q (1-\cos q)\phi_q\phi_{-q} + 2J\sum_q (1-\cos q+d)S_q^zS_{-q}^z, \tag{4}$$

with $d=A/2J$, and

$$H_4=\frac{J}{N}\sum_{q_1,q_2,q_3,q_4}\delta_{q_1+q_2+q_3+q_4,0}\Bigg\{-\frac{S(S+1)}{6}[1-\cos q_1 -\cos q_2-\cos q_3-\cos q_4+\cos(q_1+q_2)+\cos(q_1+q_3) +\cos(q_1+q_4)]\phi_{q_1}\phi_{q_2}\phi_{q_3}\phi_{q_4}-[1-\cos q_2-\cos q_3 +\cos(q_1+q_4)]S_{q_1}^z\phi_{q_2}\phi_{q_3}S_{q_4}^z + \frac{1}{6S(S+1)}[3-\cos(q_1+q_2)-\cos(q_1+q_3) -\cos(q_1+q_4)]S_{q_1}^zS_{q_2}^zS_{q_3}^zS_{q_4}^z\Bigg\}. \tag{5}$$

Hamiltonian (4) can be diagonalized by using the canonical transformation

$$\phi_q=\alpha_q(a_q^+ + a_{-q}), \quad S_q^z=i\beta_a(a_q^+ - a_{-q}), \tag{6}$$

where $\alpha_q\beta_q = 1/2$, and

$$\alpha_q=\left(\frac{1}{4S(S+1)}\frac{1-\cos q+d}{1-\cos q}\right)^{1/4}. \tag{7}$$

We obtain

$$H_2=\sum_q \hbar\omega_q(a_q^+a_q+1/2), \tag{8}$$

where

$$\hbar\omega_q=4J[S(S+1)(1-\cos q)(1-\cos q+d)]^{1/2}. \tag{9}$$

As we can see from (2) and (4) a measurement of $S^{\alpha\alpha}(q,\omega)$ $(\alpha=x,y)$ does not reduce to the observation of one single magnon of wave vector q, but involves the observation of all magnons with wave vectors between, roughly, $q-k$ and $q+k$, where k is the inverse correlation length.[1] On the contrary, a measurement of $S^{zz}(q,\omega)$ does in fact correspond to the observation of a single magnon with a much smaller linewidth. In the model discussed here, at low temperatures, the linewidth of the out-of-plane component $S^{zz}(q,\omega)$ is produced by the decay of the magnon into other magnons, by the scattering by other magnons, or, in mathematical terms, by the anharmonic terms in (4). Since these terms are functions of both ϕ and S^z we use a matrix form for the temperature-dependent Green function

$$D=\begin{bmatrix} D_{\phi\phi} & D_{\phi S} \\ D_{S\phi} & D_{SS}\end{bmatrix}, \tag{10}$$

where

$$D_{\mu\alpha}(q,\tau-\tau')=\langle T\{\psi_q^\mu(\tau)\psi_{-q}^\alpha(\tau')\}\rangle, \tag{11}$$

where $\mu,\alpha=\phi$ or S, $\psi_q^s=S_q^z, \psi_q^\phi=\phi_q$, and $0<\tau<\beta$, with $\beta=1/k_BT$. T in (11) means that the operators are arranged so that τ is decreasing from left to right. The nonperturbed (bare propagator) Green function is

$$D^0(q,i\omega_n)=\begin{bmatrix} 2\alpha_q^2\omega_q & i(i\omega_n) \\ -i(i\omega_n) & 2\beta_q^2\omega_q\end{bmatrix}\frac{1}{(i\omega_n)^2-\omega_q^2}, \tag{12}$$

where

$$D(q,i\omega_n)=\int_0^\beta d\tau e^{i\omega_n\tau}D(q,\tau), \quad \omega_n=2n\pi T. \tag{13}$$

The temperature-dependent Green function for the interacting system obeys a matrix form of Dyson's equation and can be written as

$$D(q,i\omega_n)=\begin{bmatrix} 2\alpha_q^2\omega_q+\sum_{SS} & -\omega_n-\sum_{\phi S} \\ \omega_n-\sum_{S\phi} & 2\beta_q^2\omega_q+\sum_{\phi\phi}\end{bmatrix} \times\frac{1}{[(i\omega_n)^2-\omega_q^2(1+\Delta)],} \tag{14}$$

where

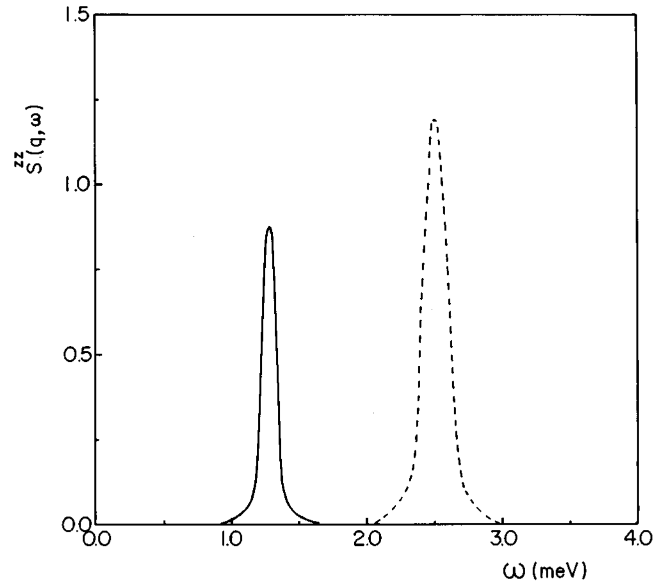

FIG. 1. The out-of-plan dynamical relaxation function in arbitrary units, as a function of ω for $T=4.7$ K and $q/\pi = 0.2$ (solid line); $q/\pi=0.3$ (dashed line).

$$\Delta=\frac{2}{\omega_q}\left(\alpha_q^2\sum_{\phi\phi}+\beta_q^2\sum_{SS}\right)+\frac{\omega_n(\Sigma_{\phi S}-\Sigma_{S\phi})}{\omega_q^2} +\frac{\Sigma_{\phi\phi}\Sigma_{SS}-\Sigma_{\phi S}\Sigma_{\phi S}}{\omega_q^2}, \tag{15}$$

and the $\Sigma_{\mu\alpha}$ are elements of a self-energy matrix. The calculation of $\Sigma_{\mu\alpha}$ follows the procedure given in Ref. 10 by making the following replacement[11] $it\rightarrow\tau$. The remaining task is the computation of the self-energy (irreducible connected) graphs which sum to give the Σ function. We have done this calculation up to the two loop level; this is the entire second order expansion. Since the calculation is standard we quote only our results for the dynamic relaxation function $S^{zz}(q,\omega)$ which is related to the temperature-dependent Green function by[11]

$$S^{zz}(q,\omega)=-\frac{4\pi}{\omega}\mathrm{Im}D_{SS}(q,\omega+i\delta). \tag{16}$$

We have calculated $S^{zz}(q,\omega)$ for the compound $CsNiF_3$ as a function of ω using Eq. (16) and in Fig. 1 we show some examples of our calculations. In Fig. 2 we show the peak position (magnon dispersion relation) as a function of the wave vector q at a temperature $T=4.2$ K. The experimental data is from Ref. 5. As we said before we fitted the experimental data by adjusting the anisotropy parameter A to $A=9.0$ K, in agreement with previous estimates.[6,8] For the peak position the second-order correction (two-loop graphs plus the second-order contribution from one-loop graphs) adds, at most, 2% to the one-loop result, and this leads us to believe that our calculation, by just going to the two-loop level, is accurate. Of course the first-order correction leads to a null linewidth. In Fig.3 we show our theoretical prediction for the OP linewidth Γ at $T=4.7$ K compared with experimental results of Kakurai, Steiner, and Dorner.[8] As pointed

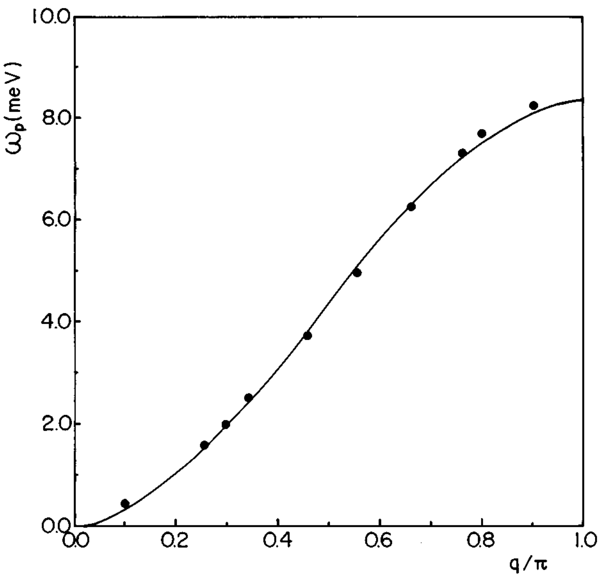

FIG. 2. Peak position as a function of the wave vector for $T=4.2$ K. The solid line is our theoretical prediction. The filled circles are experimental data from Ref. 9.

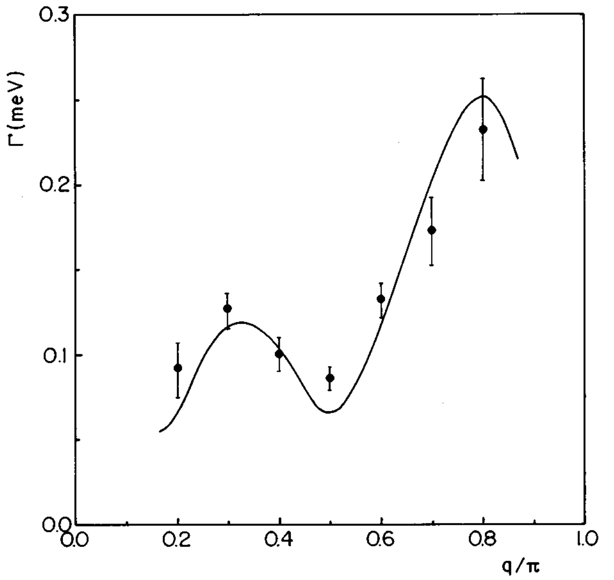

FIG. 3. q-dependence of the OP linewidth Γ at $T=4.7$ K. The solid line is our theoretical prediction. The filled circles are experimental data from Ref. 5.

out by Reiter[9] the anomalous behavior in the OP linewidth is due to a singularity in the three spin wave density of states, which are the major channels for the decay processes of the OP spin wave.

In conclusion, we have calculated the OP dynamical spin correlation function for the easy-plane one-dimensional ferromagnet, to the two-loop level. We have applied this calculation to $CsNiF_3$, and obtained the anomalous wave vector dependence in the spin wave linewidth, observed experimentally by Kakurai, Steiner, and Dorner.[8]

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