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LETTER TO THE EDITOR

Coupling between longitudinal and transverse fluctuations in a Heisenberg ferromagnet

R S Fishman† and S H Liu
Solid State Division, PO Box 2008, Oak Ridge National Lab, Oak Ridge, TN 37831, USA

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Abstract. The coupling between the longitudinal and transverse fluctuations in a spin s ferromagnet becomes significant above a crossover temperature $\bar{T} \approx T_C/s$. This coupling produces a splitting of the spin-wave resonance near the energy zJs, where z is the coordination number and J the coupling constant. We calculate the transverse mode frequencies and propose an experiment to detect the longitudinal fluctuations.

For some time, scientists (see, e.g., [1,2]) have wondered about the nature and observability of longitudinal fluctuations in a ferromagnet. The spin-wave (SW) theory developed by Dyson [3] and others [4,5] provides a wealth of predictions about the low-temperature properties of the transverse excitations. But it says nothing about the longitudinal fluctuations, which are expected to become important at higher temperatures. Although the evidence for spin-waves is abundant, longitudinal excitations have only been observed very close to the Curie temperature [6,7]. In this letter, we show that the coupling between the transverse and longitudinal fluctuations becomes significant above the temperature $\bar{T} \approx T_C/s$, where s is the spin. The longitudinal fluctuations of a pair of spins can excite a propagating, precessional mode with an energy near zJs, where J is the ferromagnetic coupling constant and z is the number of nearest neighbours in the lattice. Due to the coupling between the SW and precessional modes, the two transverse modes repel at the energy zJs. If the damping of the precessional mode is sufficiently weak, this repulsion would be observed as a splitting of the transverse resonance peak.

To evaluate the mode frequencies of a ferromagnet, we employ a systematic expansion of the transverse correlation function. This technique produces a coupling term that is exponentially small at low temperatures but becomes significant above the crossover temperature $\bar{T}$. Because the SW approximation omits this term, it neglects the coupling between the SW and precessional modes. Since this technique will be explained in greater detail in future papers [8], we briefly sketch the method here.

The Hamiltonian of the Heisenberg ferromagnet in zero field is

$$H = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

† Permanent address: Department of Physics, SU Station Box 5566, North Dakota State University, Fargo, ND 58105-5566, USA.

where $J > 0$ and the spins obey the commutation relations

$$[S_{\alpha i}, S_{\beta j}] = -\mathrm{i}\delta_{ij}\varepsilon_{\alpha\beta\gamma}S_{i\gamma} \tag{2}$$

with $\hbar = 1$. In order to calculate the correlation function and mode frequencies, we split the Hamiltonian into a mean-field (MF) part H_{eff}, a constant term H_1, and a fluctuation term H_2:

$$H = H_{\text{eff}} + H_1 + H_2 \tag{3}$$

$$H_{\text{eff}} = -zJM_0\sum_i S_{iz} \tag{4}$$

$$H_1 = \tfrac{1}{2}NzJM_0{}^2 \tag{5}$$

$$H_2 = -J\sum_{\langle i,j\rangle}\{(S_{iz} - M_0)(S_{jz} - M_0) + S_{ix}S_{jx} + S_{iy}S_{jy}\}. \tag{6}$$

The MF order parameter $M_0(T^\star) = \langle S_{1z}\rangle_{\text{MF}}$, which is a function only of $T^\star = T/zJ$ and s, is evaluated by neglecting H_2. Notice that H_2 couples the local spin fluctuations on neighbouring lattice sites. As z increases, the mean-field zJM_0 experienced by each spin becomes stronger and the coupling of fluctuations becomes weaker. So the effects of H_2 can be studied with a $1/z$ expansion about MF theory [9].

We use this decomposition of the Hamiltonian to evaluate the spin–spin correlation function

$$D(\boldsymbol{k}, \mathrm{i}\omega_n) = \sum_i \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i} D_{1i}(\mathrm{i}\omega_n) \tag{7}$$

$$D_{ij}(\mathrm{i}\omega_n) = -\int_0^\beta \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega_n\tau}\langle T_\tau S_i^+(\tau)S_j^-(0)\rangle \tag{8}$$

where $S_i^\pm = S_{ix} \pm S_{iy}$, $\omega_n = 2n\pi T$ are the Matsubara frequencies, $\beta = 1/T$, $\boldsymbol{R}_i$ are the lattice vectors with $\boldsymbol{R}_1 = 0$, T_τ is the time ordering operator, and the Heisenberg operator $A(\tau)$ is defined by

$$A(\tau) = \mathrm{e}^{\tau H}A\mathrm{e}^{-\tau H}. \tag{9}$$

The transverse mode frequencies are poles in the correlation function $D(\boldsymbol{k}, w)$, which is obtained from $D(\boldsymbol{k}, \mathrm{i}\omega_n)$ by the substitution $\mathrm{i}\omega_n \to \omega + \mathrm{i}\delta$. If the exact Hamiltonian H is replaced by the MF Hamiltonian H_{eff}, then the Matsubara correlation function is given by

$$D^{(0)}(\boldsymbol{k}, \mathrm{i}\omega_n) = D^{(0)}(\mathrm{i}\omega_n) \equiv \frac{2M_0}{\mathrm{i}\omega_n - \Delta_0} \tag{10}$$

where $\Delta_0 = zJM_0$.

More generally, the exact correlation function can be expressed as

$$D(\boldsymbol{k}, \mathrm{i}\omega_n) = \frac{D^{(0)}(\boldsymbol{k}, \mathrm{i}\omega_n)}{1 - D^{(0)}(\boldsymbol{k}, \mathrm{i}\omega_n)\Sigma(\boldsymbol{k}, \mathrm{i}\omega_n)} \tag{11}$$

where the self-energy $\Sigma(\mathbf{k}, \mathrm{i}\omega_n)$ embodies the correlation of fluctuations produced by H_2. This relation can inverted to yield the *definition* of the self-energy

$$\Sigma(\mathbf{k}, \mathrm{i}\omega_n) = \frac{1}{D^{(0)}(\mathbf{k}, \mathrm{i}\omega_n)} - \frac{1}{D(\mathbf{k}, \mathrm{i}\omega_n)}. \tag{12}$$

The correlation function may be written in the form of (11) because $D^{(0)}(\mathbf{k}, \mathrm{i}\omega_n)$ is non-zero for all $\mathbf{k}$ and all n.

To evaluate the mode frequencies, we expand the self-energy in powers of $1/z$ as

$$\frac{\Sigma(\mathbf{k}, \mathrm{i}\omega_n)}{zJ} = \sigma_0 + \frac{1}{z}\sigma_1 + \dots. \tag{13}$$

Each coefficient σ_m is a function only of the dimensionless quantities $\mathrm{i}\omega_n/zJ$, T^*, s, and dimensionless functions like

$$\gamma_{\mathbf{k}} = \frac{1}{z}\sum_{\boldsymbol{\delta}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}} \tag{14}$$

where $\boldsymbol{\delta}$ are the nearest-neighbour vectors. Since the sum in (14) runs over z different vectors, $\gamma_{\mathbf{k}}$ is of order 1 rather than of order $1/z$.

The functions σ_m are evaluated by first expanding every correlation function $D_{ij}(\mathrm{i}\omega_n)$ in powers of $1/z$. Fourier-transforming then yields the $1/z$ expansion of $D(\mathbf{k}, \mathrm{i}\omega_n)$. Finally, (12) provides the expansion of the self-energy. To evaluate σ_0, we must expand $D_{1i}(\mathrm{i}\omega_n)$ to order $1/z^m$, where $\mathbf{R}_i$ is m lattice vectors removed from $\mathbf{R}_1 = 0$. The fourier transform of (7) then sums over the $z^m/m!$ equivalent sites $\mathbf{R}_i$ oriented symmetrically about $\mathbf{R}_1 = 0$. The evaluation of σ_1 requires the $1/z^{m+1}$ correction to $D_{1i}(\mathrm{i}\omega_n)$ for all $\mathbf{R}_i$. We have also used this method [8] to calculate the static, longitudinal correlation function in the paramagnetic state. As expected, the long-range correlations diverge at the true, shifted Curie temperature [9]. A related technique has been used by Gros and Johnson [10] to evaluate the $1/z$ corrections to the self-energy of a spin 1/2 antiferromagnet at zero temperature.

Up to order $1/z$, the self-energy is given by

$$\sigma_0 = -\tfrac{1}{2}\gamma_{\mathbf{k}} \tag{15}$$

$$\sigma_1 = \frac{\mathrm{i}\omega_n}{2zJ}\frac{M_1}{M_0^2} + \frac{1}{2M_0^2}(1-\gamma_{\mathbf{k}})\left(\frac{\Delta_0 f_1}{\mathrm{i}\omega_n - \Delta_0} + f_2\right) \tag{16}$$

where

$$f_1(T^*) = 2\langle \tilde{S}_{1z}^2 \rangle_{\mathrm{MF}} \tag{17}$$

$$f_2(T^*) = \frac{1}{T^*}\left\{\langle \tilde{S}_{1z}^2 \rangle_{\mathrm{MF}}^2 + \tfrac{1}{4}\langle S_1^+ S_1^- \rangle_{\mathrm{MF}} \langle S_1^- S_1^+ \rangle_{\mathrm{MF}}\right\} \tag{18}$$

and $\tilde{S}_{1z} = S_{1z} - M_0$. To order $1/z$, the corrected order parameter $M = \langle S_{1z} \rangle$ is given by $M_0 + M_1/z$, where $M_1(T^*)$ was previously calculated in [9].

Using (11) for the correlation function, we arrive at the final result

$$D(\mathbf{k}, \mathrm{i}\omega_n) = 2M\left\{\mathrm{i}\omega_n - \Delta(1-\gamma_{\mathbf{k}}) - \frac{(zJ)^2}{z}(1-\gamma_{\mathbf{k}})\left(\frac{1}{\mathrm{i}\omega_n - \Delta}f_1 + \frac{1}{\Delta}f_2\right)\right\}^{-1} \tag{19}$$

where $\Delta = zJM$ is now proportional to the corrected order parameter. Replacing $i\omega_n$ by $\omega + i\delta$ and setting $D(\boldsymbol{k},\omega)^{-1} = 0$ yields the mode frequencies.

To zero order in $1/z$, the correlation function has a pole at $\omega = \Delta_0(1-\gamma_{\boldsymbol{k}})$, which is the result of the random phase approximation [11] (RPA) for the SW frequency. Aside from renormalizing the order parameter, the first-order self-energy σ_1 contains two correction terms, f_1 and f_2. The f_2 term is produced by the interaction between pairs of spin-waves. This term is also contained in the SW theory of Dyson [3] and Maleev [4] (DM). So in the absence of the f_1 term in the self-energy, the corrected SW frequency of (19) agrees with the DM result.

Unlike the f_2 term, f_1 introduces new dynamics into the correlation function. Including the f_1 term in σ_1, we find the astonishing result that the correlation function now has two poles: one close to the DM frequency, the other close to Δ. The correction term f_1 is produced by the coupling between the longitudinal and transverse fluctuations. At low temperatures, when longitudinal fluctuations are suppressed, $f_1 \propto e^{-zJs/T}$ can be neglected. But above the crossover temperature [12] $\bar{T} \approx 0.2zJs$, longitudinal fluctuations are possible and f_1 is significant.

The mode frequencies are plotted in figure 1 for a cubic lattice with $s = 1/2$, $z = 6$, and $T^*/s(s+1) = 0.15$. At very low temperatures, the SW frequency $zJs(1-\gamma_{\boldsymbol{k}})$ and the precessional frequency zJs cross without repelling. But above $\bar{T}$, the coupling term f_1 causes the two transverse branches to repel at the mode-crossing point $\gamma_{\boldsymbol{k}} = 0$. The magnitude of the splitting between the branches at $\gamma_{\boldsymbol{k}} = 0$ is of order $1/\sqrt{z}$ rather than of order $1/z$.

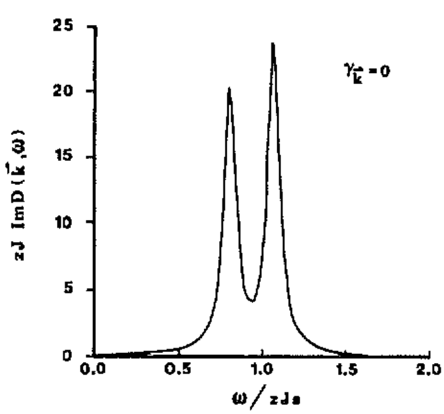

Figure 1. The mode frequencies ω/zJs versus $\gamma_{\boldsymbol{k}}$ for $s = 1/2$, $z = 6$, and $T^*/s(s+1) = 0.15$. The spin-wave frequency with f_1 set to zero is plotted as the dashed line.

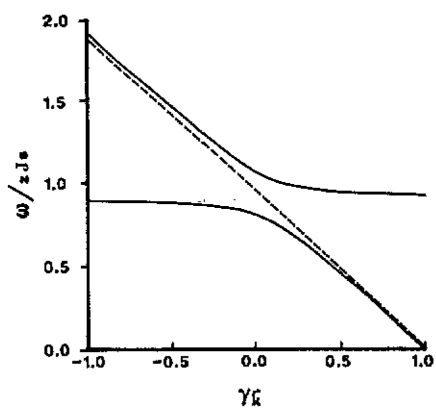

Figure 2. The imaginary part of $D(\boldsymbol{k},\omega)$ versus ω/zJs for $\gamma_{\boldsymbol{k}} = 0$ and $\Gamma = zJf_1$. All other parameters as in figure 1.

Because it alters the spin commutation relations of (2), the SW approximation mishandles the subtle relationship between the longitudinal and transverse fluctuations. When the spin operators are replaced by the creation and annihilation operators of the SW approximation, the coupling term f_1 vanishes. Setting f_1 to zero would eliminate the second pole in the correlation function and yield the DM frequency plotted as the dotted line of figure 1.

The precessional mode is excited by longitudinal fluctuations on neighbouring lattice sites. A longitudinal fluctuation forces the local spin to precess around the mean field zJM with the precession frequency Δ rather than with the SW frequency ω_k. Because this local fluctuation couples with the surrounding spins, the precession propagates through the lattice with a frequency which is shifted from Δ by dispersion. When ω_k is very different from Δ, the coupling between the SW and precessional modes is weak. But when ω_k is close to Δ, the mixing between the SW and precessional modes induces a large shift in both of their energies.

We must carefully distinguish the precessional mode from longitudinal excitations, which are dispersionless and have zero frequency [1,6–8]. Longitudinal excitations have been directly observed [6,7] only very close to the Curie temperature. Unlike longitudinal excitations, the precessional mode is dispersive and propagates through the lattice: to order $1/z$ in the self-energy, the mode couples each site with every other site in the lattice. Although induced by the longitudinal fluctuations of a pair of spins, the precessional mode is fundamentally a transverse excitation of the lattice; above $\bar{T}$, the spectral weight of the transverse correlation function is shared by the precessional and SW modes.

Our results for the mode frequencies assume that the $1/z$ expansion of the self-energy converges above $\bar{T}$. Because spin-waves destroy the long-range order of the spins in two dimensions, the $1/z$ expansion about the ordered state $\langle S_{iz}\rangle = M_0$ is justified only in three dimensions. Although we cannot prove that σ_1/z provides the dominant correction to the zero-order self-energy σ_0 in three dimensions, there are strong indications that the $1/z$ expansion yields sensible results. First, σ_0 generates the expected, lowest-order RPA frequency. Even this calculation involves the non-trivial summation of the $1/z^m$ correction to every correlation function. Second, each term in σ_1/z can be interpreted physically. While the f_2 term is produced by the interactions between spin-waves, as found by Dyson [3], the f_1 term is produced by the coupling between transverse and longitudinal fluctuations.

Unfortunately, our expansion technique cannot be used to calculate the damping of the SW and precessional modes above $\bar{T}$. Because the widths Γ_1 and Γ_2 of the SW and precessional modes are non-analytic functions of $1/z$, they vanish to any finite order in the expansion. As argued by Vaks, Larkin, and Pikin [1], the damping of the transverse modes at high temperatures is dominated by the coupling between the transverse and longitudinal fluctuations. Hence, it seems rather likely that both Γ_1/J and Γ_2/J are of the same order as the coupling term f_1. In fact, the expression for Γ_1 calculated by Vaks *et al* is indeed a non-analytic function of $1/z$ and proportional to Jf_1. Although their result is probably not valid above $\bar{T}$, it still serves as a useful estimate for the damping of the modes.

Although Γ_1 and Γ_2 are generally quite different, they become equal near the mode-crossing point. So when $\gamma_k \approx 0$, we may replace ω by $\omega - \mathrm{i}\Gamma$ in the correlation function and use the result of Vaks *et al* to estimate $\Gamma = zJf_1$. In figure 2, we plot the imaginary part of $D(k,\omega)$ versus ω for $\gamma_k = 0$. The splitting of the spin-wave resonance into two peaks can be clearly seen. Since the SW and precessional modes are completely mixed at this point in k space, neutron scattering measurements will couple to both branches. As $|\gamma_k|$ increases, the mixing of the modes decreases and the precessional peak becomes weaker. While the precessional mode survives when $\gamma_k = -1$, its residue vanishes in the long-wavelength limit $k \to 0$ and $\gamma_k \to 1$. For $s = 1/2$, both peaks should be observable even for $|\gamma_k|$ as large as $1/3$. But for larger values of the spin, the mode splitting may be observable only for rather small values of $|\gamma_k|$.

The mode repulsion might be detectable in a narrow window of temperatures. If $T < \bar{T}$, both f_1 and the spectral weight of the precessional mode are negligible. But if the temperature is sufficiently high that Γ is of the same order as Δ, then only the SW branch will be observable. Hence, the best temperature to observe the splitting is slightly above the crossover temperature $\bar{T} \approx 0.2zJs$ so that f_1 is significant but Γ is still small compared with Δ.

However, if the precessional mode is overdamped so that $\Gamma_2 \gg \Delta$, then the mode splitting may be impossible to observe at any temperature. This seems to be the case for EuO [13], which has a spin of $7/2$ and a coordination number of $z = 12$. But even if the splitting is not observable, the attenuation of the transverse resonance should become anomalously large in the immediate vicinity of the mode-crossing point. It may also be possible to observe the systematic deviations of the SW frequencies from the predictions of Dyson and Maleev. Like the mode splitting, these effects should become more pronounced with smaller spin.

To summarize, we have proposed a method to study the effects of longitudinal fluctuations in a ferromagnet. A pair of longitudinal fluctuations may excite a precessional mode of the lattice. Above the crossover temperature $\bar{T}$ and near the mode-crossing point $\gamma_k = 0$, the coupling between the precessional and SW modes produces a splitting of the transverse resonance peak. If the damping of the precessional mode is sufficiently weak, this splitting may be observable through neutron scattering measurements.

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