Classical Ferromagnetic Heisenberg Chain in a Magnetic Field

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The dynamics of classical ferromagnetic Heisenberg chains in a magnetic field is investigated. Contrary to previous theories, in the longitudinal spectral shapes temperature is found to play a crucial role through a dynamical spin-energy coupling whose effect is competitive with the field. Thermal disorder ultimately causes a nearly isotropic situation, leading to a new interpretation of the features of recent computer experiments.

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Recent computer simulations on classical Heisenberg ferromagnetic chains[1] in the presence of a magnetic field have shown several interesting features which have caused considerable discussions.[2-5] The spectrum of the longitudinal magnetization fluctuations $\langle S_{-k}^z S_k^z(t)\rangle$ $(k\neq 0)$ is dramatically affected by the field, particularly in the case of intermediate wave vectors where even two-peaked structures may appear. The lower-frequency peak was referred[1] to as due to a "second-magnon"–like excitation, while the other one was ascribed to usual spin waves modified by the field. Afterwards, theoretical interpretations[2,3] have been worked out by using a multivariable Mori approach in which the coupling between energy and spin fluctuations was invoked as due to the field. As a final result of these theories, spectral shapes where the temperature does not play a determinant role are found.

In this paper we will instead show that the spectral shapes are crucially influenced by thermal effects which control the dynamic spin-energy coupling and that this thermally activated coupling arises quite naturally in the framework of an interacting spin-wave theory. Moreover, we find that the peaks at different frequencies can be simply interpreted as due to the competition between temperature and magnetic field. Temperature introduces "disorder" in the dynamics of the system: For moderate fields and intermediate wave vectors the physics is essentially that of an isotropic one-dimensional (1D) system at a lower temperature. In this respect the "low-frequency" peak is a simple consequence of this thermally induced isotropy and interpretations based on "second-magnon" concepts appear to be unjustified.

The features of the spectrum of $\langle S_{-k}^z S_k^z(t)\rangle$ in the presence of a magnetic field H can be studied by means of the usual Dyson-Maleev transformation to Bose operators a_k, $a_k^\dagger$. With the omission of constant terms, the boson Hamiltonian of the 1D system reads

$$\mathcal{H}=\sum_k(\Omega_k+g\mu_B H)a_k^\dagger a_k-\frac{J}{N}\sum_{qpq'p'}\delta_{q+p,q'+p'}(\gamma_{q-q'}-\gamma_{q'})a_q^\dagger a_p^\dagger a_{q'}a_{p'}\,, \tag{1}$$

where $\gamma_k=\cos k$ in lattice units and $\Omega_k=2JS(1-\gamma_k)$. The fluctuation of the quantity S_k^z is given by

$$\hat{S}_k^z\equiv S_k^z-\langle S_k^z\rangle=-N^{-1/2}\sum_q a_{k+q}^\dagger a_q. \tag{2}$$

It is also convenient to introduce the space Fourier transform E_k of the exchange energy of a spin with its neighbors. The fluctuation of E_k is found to be

$$\hat{E}_k\equiv E_k-\langle E_k\rangle\simeq -N^{-1/2}S\sum_q(1+\gamma_k-\gamma_q-\gamma_{k+q})a_{k+q}^\dagger a_q\,, \tag{3}$$

in which quartic terms in the Bose operators have been neglected.

We now evaluate the spectrum $\langle\hat{S}_{-k}^z\hat{S}_k^z\rangle_\omega$ by Zubarev Green's-function techniques, i.e., through the equation of motion of $\langle\langle a_{k+q}^\dagger a_q;a_{-k+q'}^\dagger a_{q'}\rangle\rangle_E$. Decoupling higher-order Green's functions we get the following equation of motion which contains all the leading temperature terms in the classical case:

$$\begin{aligned}(E+\overline{\Omega}_{k+q}-\overline{\Omega}_q)&\langle\langle a_{k+q}^\dagger a_q;a_{-k+q'}^\dagger a_{q'}\rangle\rangle_E\\ &=(1/2\pi)(n_{k+q}-n_q)\delta_{q',k+q}-(2J/N)(n_{k+q}-n_q)\sum_p(\gamma_k-\gamma_{k+q}-\gamma_p+\gamma_{q-p})\langle\langle a_{k+p}^\dagger a_p;a_{-k+q'}^\dagger a_{q'}\rangle\rangle_E,\end{aligned} \tag{4}$$

where $n_q=\langle a_q^\dagger a_q\rangle$ and $\overline{\Omega}_q=\alpha(T)\Omega_q$ is the Hartree-Fock renormalized magnon frequency. If the last term were ignored and $\alpha(T)=1$, we would get a "free-boson" result which is a reasonable approximation at very low temperatures. However, at finite temperatures (like those, $T^* \equiv K_B T/JS^2 = 0.3$, used in the simulations) this term cannot be neglected as it is of the same order as the Hartree-Fock correction. For the 1D case the exact solution of the integral equation (4) can be found in a relatively straightforward way. Here we only report the result for $g_k(E) \equiv \langle\langle \hat{S}_k^z; \hat{S}_{-k}^z \rangle\rangle_E$ which includes all the main temperature effects:

$$g_k(E) = \frac{g_k^{(0)}(E) + 4\pi J\{[g_k^{(0)}(E)]^2 - [h_k^{(0)}(E)]^2 - [t_k^{(0)}(E)]^2\}}{1 + 4\pi J(1+\gamma_k)[g_k^{(0)}(E) - h_k^{(0)}(E)] + \sin k\, t_k^{(0)}(E)}, \tag{5}$$

where

$$g_k^{(0)}(E) = (2\pi N)^{-1}\sum_q D_{kq}(E), \quad h_k^{(0)}(E) = (2\pi N)^{-1}\sum_q \gamma_q D_{kq}(E),$$
$$t_k^{(0)}(E) = (2\pi N)^{-1}\sum_q \sin q D_{kq}(E), \quad D_{kq}(E) = (n_{k+q} - n_q)(E + \overline{\Omega}_{k+q} - \overline{\Omega}_q)^{-1}. \tag{6}$$

The quantity $g_k^{(0)}(E) = \langle\langle \hat{S}_k^z; \hat{S}_{-k}^z \rangle\rangle_E^{(0)}$ with $\alpha(T) = 1$ represents the free-boson approximation for $g_k(E)$. The thermal corrections in the numerator yield small changes in the spectra but have been found to be important for correctly describing the static quantities at finite temperatures.[6] It is important to observe that with use of Eq. (3) the denominator of Eq. (5) can be written as $1 + (4\pi J/S)\langle\langle \hat{E}_k; \hat{S}_{-k}^z \rangle\rangle_E^{(0)}$. Therefore the physical quantity which rules the behavior of the system at finite temperatures is the dynamic coupling between spin and energy fluctuations. Temperature is thus crucial for affecting the spectral shape through this thermally activated spin-energy coupling. In the classical 1D case all these quantities can be analytically evaluated. If we let $E = \omega + i0^+$ and $x = \omega/JS\alpha(T)$, the quantity $g_k^{(0)}(E)$ for $x^2 < 4b_k^2 = 16\sin^2(k/2)$ is given by

$$2\pi \operatorname{Re} g_k^{(0)}(x) = (T^*/J\alpha^2) b_k^2 (h_T + 2)[x^2 - b_k^2(K_T^2 + b_k^2)][K_T D(k,x)]^{-1},$$
$$2\pi \operatorname{Im} g_k^{(0)}(x) = (T^*/J\alpha^2) b_k^2 x [x^2 - b_k^2(K_T^2 + 8 - b_k^2)][D(k,x) g(k,x)]^{-1}, \tag{7}$$

where $h_T = h/\alpha = g\mu_B H/JS\alpha$, $K_T^2 = h_T(h_T + 4)$, $\alpha = \alpha(T) = 1 - [T^*/2\alpha(T)](1 - h_T/K_T)$ and $g(k,x) = (4b_k^2 - x^2)^{1/2}$. Moreover,

$$D(k,x) = x^4 + b_k^2[2K_T^2 - b_k^2(K_T^2 + 2)]x^2 + b_k^4(K_T^2 + b_k^2)^2. \tag{8}$$

For $x^2 > 4b_k^2$ all integrals in (6) are real and do not contribute to the spectrum. In the case $\alpha(T) = 1$ Eqs. (7) have already been derived by Lovesey.[3] The unperturbed spectrum is proportional to $\operatorname{Im} g_k^{(0)}(x)/x$ and is seen to diverge at a frequency $x = \pm 2b_k$. This divergence derives from the factor $\{g(k,x)\}^{-1}$ and is due to a singularity in the two-magnon density of states. It appears in many 1D problems and has been discussed also recently.[4,7]

At finite temperature the effect of the dynamic spin-energy coupling $C_k^{(0)}(E) = S^{-1}\langle\langle \hat{E}_k; \hat{S}_{-k}^z \rangle\rangle_E^{(0)}$ must be considered. Letting $E = \omega + i0^+$ we find

$$2\pi \operatorname{Re} C_k^{(0)}(x) = -(T^*/J\alpha^2) 2\sin^2 k (h_T/K_T)[x^2(h_T + 3) + b_k^2(K_T^2 + b_k^2)][D(k,x)]^{-1},$$
$$2\pi \operatorname{Im} C_k^{(0)}(x) = -(T^*/J\alpha^2) 2\sin^2 k x [x^2(h_T + 1) + b_k^2(h_T^2 - b_k^2)][D(k,x) g(k,x)]^{-1}. \tag{9}$$

These terms remove the square-root singularity present in the unperturbed result. This removal follows from the nonperturbative solution of the integral equation (4). It is interesting to observe that in other 1D problems similar removals have been associated to bound-state effects.[7] We also note that (i) both parts of $C_K^{(0)}(x)$ are proportional to T and (ii) the imaginary part does not vanish even when we let $h_T \to 0$.

By use of the classical spectral theorem the spectrum $\langle \hat{S}_{-k}^z \hat{S}_k^z \rangle_\omega$ is finally found to be

$$J\langle \hat{S}_{-k}^z \hat{S}_k^z \rangle_x = S \frac{b_k^2}{\pi\alpha}\left(\frac{T^*}{\alpha}\right)^2 g(k,x) \frac{b_k^2(K_T^2 + 8 - b_k^2) - x^2 - (T^*/\alpha^2 K_T) P(k,x) + (T^*/\alpha^2 K_T)^2 8\sin^2 k}{g^2(k,x)[D(k,x) - (T^*/\alpha^2 K_T) Q(k,x)] + (T^*/\alpha^2 K_T)^2 R(k,x)}, \tag{10}$$

where

$$P(k,x) = (h_T + 2) g^2(k,x) + 8\sin^2 k, \quad R(k,x) = (8\sin^2 k)^2 h_T (x^2 + h_T b_k^2),$$
$$Q(k,x) = (8\sin^2 k) h_T[(h_T + 3)x^2 + b_k^2(K_T^2 + b_k^2)]. \tag{11}$$

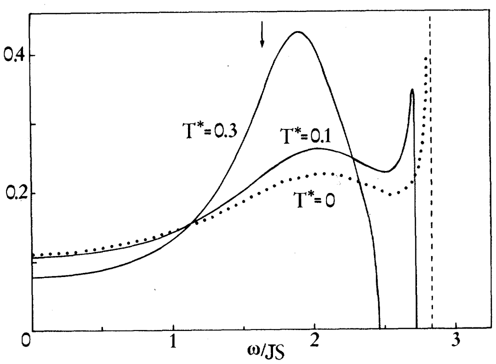

FIG. 1. Temperature dependence of the spectra for $k = 0.5\pi$, $h = 0.2$. The dotted line is the unperturbed free-boson result. Here and in the following figures all amplitudes have been normalized to the respective values of the $t = 0$ correlation function, and the arrow indicates the peak position in the isotropic system.

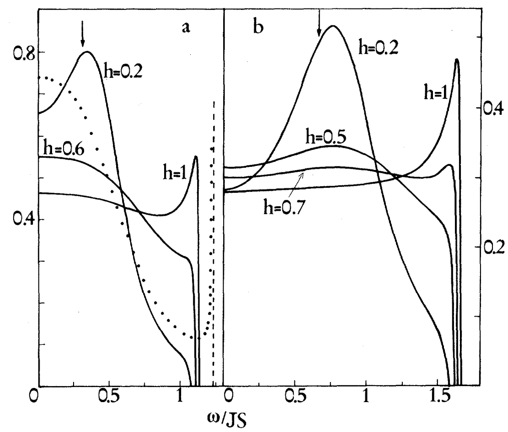

FIG. 2. Field dependence of the spectra for $T^* = 0.3$ for (a) $k = 0.2\pi$ and (b) $k = 0.3\pi$. The dotted line in (a) is the unperturbed free-boson result for $h = 0.2$ and $T^* = 0$.

It is easily seen that a low temperatures and in the limit $h_T \to 0$, Eq. (10) leads to a Lorentzian shape with peak frequency determined by the vanishing of $D(k,x)$, namely $\omega_{\text{peak}} = \Omega_k(1 - T^*/2)$ and with halfwidth $T^*JS\sin k$, i.e., the values found by Reiter and Sjölander.[8]

Our theoretical normalized spectra at several values of T^*, magnetic field h, and wave vector k are reported in Figs. 1 and 2. Figure 1 shows the temperature dependence of the spectra for a moderate field, $h = 0.2$ and $k = 0.5\pi$. The unperturbed result exhibits the expected singularity, together with a broad maximum connected with the minimum of $D(k,x)$. At $T^* = 0.1$ the spin-energy coupling removes the singularity leaving as a remnant of it a narrow peak; the other peak is now more well defined. At $T^* = 0.3$ the thermally induced disorder is sufficient for making the dynamics of the system similar to that present in an isotropic 1D system at a slightly lower effective temperature because of the competing presence of the field. The previous lower-frequency peak is now the dominant feature of the spectrum and its frequency is very near that of the isotropic case. Any trace of the "free-boson" singularity is lost.

The effects of the field on the spectra are shown in Fig. 2 for $T^* = 0.3$ and (a) $k = 0.2\pi$ and (b) 0.3π. As the ordering action of the field decreases, the isotropiclike peak arises, while the peak due to the singularity of two-magnon density of states disappears. Contrary to the situation in Fig. 1, now the free-boson result for $k = 0.2\pi$ does not show any low-frequency structure: For this low wave vector the effect of even a small field ($h = 0.2$) is sufficient to overcome the exchange contribution. This change of the spectrum with field is in agreement with the published simulation experiments[1] as well as with more recent computer data.[9] The transition from one type of regime to the other is clearly shown also for $k = 0.3\pi$, where, moreover, for $h = 0.7$ a two-peaked structure is present, in qualitative agreement with the simulation data at $T^* = 0.3$ and in this range of intermediate wave vectors. Here it is apparent that the low-frequency peak is due to the onset of a nearly isotropic situation.

As the wave vector increases in the second half of the Brillouin zone the dynamical spin-energy coupling decreases and eventually vanishes at $k = \pi$, where the only feature of the spectrum is the square-root singularity due to renormalized free bosons.

Finally we note that in our theory we have neglected damping terms in the boson propagators. The main effect of such terms, surely of higher order in temperature, is to broaden the sharp features remnant of the square-root singularity at the end of the spectrum and in particular to give rise to a high-frequency tail.

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