Low-temperature properties of layered Heisenberg ferromagnets

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Spin-wave theory is used to study the effects of interlayer coupling on the properties of layered Heisenberg ferromagnets with $S=\frac{1}{2}$. The asymptotic expressions of magnetization and specific heat with temperature and interlayer coupling strength ($J_\perp$) are given in two low-temperature regimes distinguished by a characteristic temperature $T_0=2J_\perp/k_B$. It is shown that the interlayer coupling, though very small, is essential if long-range order at nonzero temperature is to exist.

Much interest in the study of magnetic materials has focused on the properties of layered magnetic systems.[1] The recent discovery of copper oxide high-T_c superconductors with quasi-two-dimensional magnetic properties in their parent materials–which is a case in point—greatly stimulates further studies in this field. Because it has been rigorously proved by Mermin and Wagner[2] that there can be no long-range order at any nonzero temperature for two-dimensional isotropic systems, while on the other hand, layered materials with extremely weak interlayer coupling are found to exhibit long-range order at finite nonzero temperatures,[3,4] interlayer coupling must play an important role in the stabilization of three-dimensional order in layered magnetic systems.

For layered antiferromagnets, the dependences of sublattice magnetization[5] and specific heat[6] on the interlayer coupling strength have been found for low temperatures; the Néel temperature is zero in the two-dimensional case ($J_\perp=0$).[7] For layered ferromagnets, the dependence of the Curie temperature on the interlayer coupling strength is similar to that of the Néel temperature;[8] Colpa's numerical work[9] shows the effect of interlayer coupling strength on the specific heat to some extent, but his analytical expression is not entirely satisfactory for describing the effect. Because the relationship between magnetization and interlayer coupling strength at low temperatures merits further studies, we consider in detail the effects of the interlayer coupling strength on the magnetization and specific heat in layered ferromagnets with $S=\frac{1}{2}$, using numerical and analytical methods. For simplicity we start with a simple-cubic-lattice Heisenberg model with layer and interlayer lattice parameters, respectively, a and c. The model Hamiltonian is

$$H=-\sum_{\langle i,j\rangle} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j , \tag{1}$$

where the summation is taken over all nearest-neighbor sites $\langle i,j\rangle$. We also define J_{ij} for convenience:

$$J_{ij}=\begin{cases} J & \text{if sites } i \text{ and } j \text{ are in the same layer} , \\ J_\perp & \text{if sites } i \text{ and } j \text{ are in two nearest-neighbor layers} . \end{cases} \tag{2}$$

After performing the Holstein-Primakoff transformation on $\mathbf{S}_i$ and $\mathbf{S}_j$ and introducing the spin-wave operators $a_k^\dagger$ and a_k, we may rewrite Eq. (1) in harmonic-oscillator form

$$H=-\frac{(2+\delta)NJ}{2}+\sum_k \hbar\omega_k a_k^\dagger a_k , \tag{3}$$

where N is the total number of the lattice sites, $\delta=J_\perp/J$, and $\hbar\omega_k$ is given by the dispersion relation

$$\hbar\omega_k=2J[2+\delta-\cos(k_x a)-\cos(k_y a)-\delta\cos(k_z c)] . \tag{4}$$

Thus, we can calculate such physical quantities of system as the magnetization, internal energy, and specific heat, and so on.

The magnetization per site m (the unit is taken to be $g\mu_B$) is given by

$$\begin{aligned} m&=S-\frac{1}{N}\sum_k[\exp(\beta\hbar\omega_k)-1]^{-1} \\ &=\tfrac{1}{2}-\sum_{n=1}^{\infty}\exp[-2(2+\delta)n\beta J][I_0(2n\beta J)]^2 I_0(2\delta n\beta J) , \end{aligned} \tag{5}$$

where $\beta=1/k_BT$ and I_0 is the zeroth-order Bessel function of imaginary argument. In deriving Eq. (5), we first expanded the Bose distribution function in powers of the exponential, replaced the summation over k by an integral over k, and performed the integral.

Similarly, by use of the definition $E=\langle H\rangle/N$, we may obtain the internal energy per site,

$$\begin{aligned} E/2J&=-\frac{2+\delta}{4}+\frac{1}{2JN}\sum_k\hbar\omega_k[\exp(\beta\hbar\omega_k)-1]^{-1} \\ &=-\frac{2+\delta}{4}+\sum_{n=1}^{\infty}\exp[-2(2+\delta)n\beta J]I_0(2n\beta J) \\ &\quad\times\{2I_0(2\delta n\beta J)[I_0(2n\beta J)-I_1(2n\beta J)]+\delta I_0(2n\beta J)[I_0(2\delta n\beta J)-I_1(2\delta n\beta J)]\} , \end{aligned} \tag{6}$$

where I_1 is the first-order Bessel function of imaginary argument. From $C_m = \partial E/\partial T$ and Eq. (6), we obtain the specific heat per site,

$$C_m/k_B = \frac{1}{N}\sum_k (\beta\hbar\omega_k)^2 \exp(\beta\hbar\omega_k)[\exp(\beta\hbar\omega_k)-1]^{-2} . \tag{7}$$

We calculate numerically the magnetization and specific heat per site for various temperatures and interlayer coupling strengths based on Eqs. (5) and (7). The results are plotted in Figs. 1 and 2, respectively. It is shown that the Curie temperature (the intercept of a curve with the abscissa axis in Fig. 1) approaches zero at a very slow rate as the interlayer coupling strength $J_\perp = \delta J$ approaches zero. Although the Curie temperature that we obtained is very rough because of the simple method that we used, its functional dependence on δ is in agreement with that expressed asymptotically for small values of δ.[8] As to the specific-heat curves in Fig. 2, they asymptotically approach closely the curve corresponding to the two-dimensional case ($\delta=0$) for small δ.

Now we investigate the behavior of the magnetization and specific heat at low temperatures, using an analytical method. The low-temperature regime, which is defined by $2\beta J \gg 1$ (or $T \ll T_1 = 2J/k_B$), may be divided into two parts according to the values of $J_\perp$: the first part is $T \ll T_0 \le T_1$; the second is $T_0 \ll T \ll T_1$. Here T_0 is defined as $T_0 = 2J_\perp/k_B$.

(a) For the first low-temperature regime $T \ll T_0 \le T_1$, which corresponds to the three-dimensional case, we obtain, employing asymptotic expressions of Bessel functions from Eq. (5),

$$m = \frac{1}{2} - \frac{1}{(2\pi)^{3/2}}\left[\frac{T}{T_1}\right]\left[\frac{T}{T_0}\right]^{1/2} \times \left[\zeta\left[\frac{3}{2}\right] + \frac{2\delta+1}{8}\zeta\left[\frac{5}{2}\right]\left[\frac{T}{T_0}\right] + \cdots\right] , \tag{8}$$

where ζ is the Riemann zeta function. The leading term due to thermal spin-wave excitation is just the well-known $T^{3/2}$ law of Bloch describing the deviation from the maximum value at $T=0$. Similarly, from Eq. (6), we obtain

$$E/2J = -\frac{2+\delta}{4} + \frac{3}{2(2\pi)^{3/2}}\left[\frac{T}{T_1}\right]^2\left[\frac{T}{T_0}\right]^{1/2} \times \left[\zeta\left[\frac{5}{2}\right] + \frac{5(2\delta+1)}{24}\zeta\left[\frac{7}{2}\right]\left[\frac{T}{T_0}\right] + \cdots\right] . \tag{9}$$

The specific heat per site is found to be

$$C_m/k_B = \frac{15}{4(2\pi)^{3/2}}\left[\frac{T}{T_1}\right]\left[\frac{T}{T_0}\right]^{1/2} \times \left[\zeta\left[\frac{5}{2}\right] + \frac{7(2\delta+1)}{24}\zeta\left[\frac{7}{2}\right]\left[\frac{T}{T_0}\right] + \cdots\right] , \tag{10}$$

of which the leading term in $T^{3/2}$ also reflects the three-dimensional magnetic character of the system. One finds readily that, for δ equal to 1, the magnetization, internal energy, and specific heat per site are just those given by the long-wavelength approximation for the simple cubic lattice. The temperature regime reflecting the three-dimensional character of the system becomes smaller with decreasing interlayer coupling strength, as can be seen from the definition of T_0 and the asymptotic conditions; when interlayer coupling strength drops below a certain value, the regime approaches zero and the system actually exhibits quasi-two-dimensional, rather than three-dimensional properties. So the above given expressions are not appropriate for discussions of the quasi-

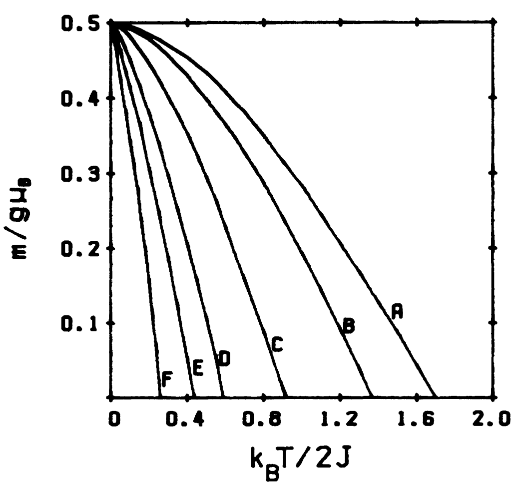

FIG. 1. Temperature dependence of the magnetization per site for several values of the interlayer coupling strength: $\delta=1.0$ (curve A), $\delta=0.5$ (curve B), $\delta=0.1$ (curve C), $\delta=0.01$ (curve D), $\delta=0.001$ (curve E), and $\delta=0.00001$ (curve F).

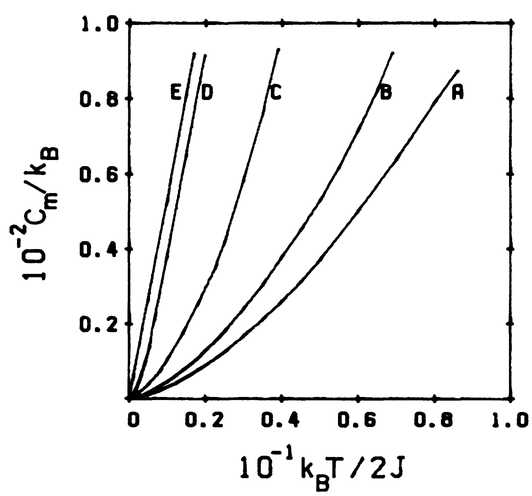

FIG. 2. Temperature dependence of the specific heat per site for several values of the interlayer coupling strength: $\delta=1.0$ (curve A), $\delta=0.5$ (curve B), $\delta=0.1$ (curve C), $\delta=0.01$ (curve D), and $\delta=0.0$ (curve E).

two-dimensional case. The second low-temperature regime is precisely this case.

(b) For the second low-temperature case, $T_0 \ll T \ll T_1$, which describes the quasi-two-dimensional case, we first transform $I_0(2\delta n\beta J)$ and $I_1(2\delta n\beta J)$ into integrals respectively in Eqs. (5) and (6). Employing asymptotic conditions and summation over n, we find, after a lengthy integration,

$$m=\frac{1}{2}-\frac{1}{2\pi}\frac{T}{T_1}\ln\left[\frac{2T}{T_0}\right]+\cdots \quad (11)$$

and

$$E/2J=-\frac{2+\delta}{4}+\frac{\zeta(2)}{2\pi}\left[\frac{T}{T_1}\right]^2-\frac{\delta}{2\pi}\frac{T}{T_1}+\cdots . \quad (12)$$

The specific heat is found to be

$$C_m/k_B=-\frac{\delta}{2\pi}+\frac{\zeta(2)}{\pi}\frac{T}{T_1}+\cdots . \quad (13)$$

With these expressions, we can discuss the quasi-two-dimensional case. From Eq. (11), we find that the second term diverges logarithmically as T_0 (or $J_\perp$) tends to zero. As a result, in the two-dimensional case there is no long-range order above zero temperature. In other words, in order to get ferromagnetic ordering at finite, nonzero temperatures, $J_\perp$ must be nonzero. The argument is very similar to that for quasi-two-dimensional antiferromagnets.[5] Because the first term in Eq. (13) is much smaller than the second term, the specific-heat curves for small values of δ are very close to that of the two-dimensional case ($\delta=0$), which is a straight line. For $\delta=0$, we have

$$C_m/k_B=\frac{\zeta(2)}{\pi}\frac{T}{T_1}\approx 0.262\frac{k_BT}{J} , \quad (14)$$

which is just the result of the long-wavelength approximation for two-dimensional ferromagnets.[9]

In summary, at low temperatures ($T \ll 2J/k_B$), as the interlayer coupling strength tends to zero, the correction due to thermal spin-wave excitation to the magnetization diverges logarithmically at finite, nonzero temperatures. For weak interlayer coupling ($0<J_\perp \ll J$), the temperature dependences of the magnetization and specific heat initially show three-dimensional behaviors as the temperature increases from $T=0$ ($0\le T \ll 2J_\perp/k_B$), but then show quasi two-dimensional behaviors as the temperature moves into the second regime ($2J_\perp/k_B \ll T \ll 2J/k_B$). As the interlayer coupling strength $J_\perp$ approaches J ($J_\perp \sim J$), only three-dimensional behaviors are retained.

[1]L. J. de Jongh and A. R. Miedema, Adv. Phys. **23**, 1 (1974).

[2]N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).

[3]L. J. de Jongh, P. Bloembergen, and J. H. P. Colpa, Physica **58**, 305 (1972).

[4]S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).

[5]A. Singh, Z. Tešanović, H. Tang, G. Xiao, C. L. Chien, and J. C. Walker, Phys. Rev. Lett. **64**, 2571 (1990).

[6]G. Z. Wei and A. Du (unpublished).

[7]C. M. Soukoulis, S. Datta, and Y. H. Lee, Phys. Rev. B **44**, 446 (1991).

[8]S. H. Liu, J. Magn. Magn. Mater. **82**, 294 (1989).

[9]J. H. P. Colpa, Physica **57**, 347 (1972).