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Monte Carlo Study of Layered Heisenberg Ferromagnet

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Monte Carlo simulation was employed to study the phase transition in the classical Heisenberg ferromagnet with variable interlayer interactions. The measured transition temperatures show a strong logarithmic dependence on J/J', where J and J' are the intralayer and the interlayer exchange interaction, respectively. The results were compared with the theoretical expectations and an empirical formula for the critical coupling was btained.

Key words : Monte Carlo, Heisenberg magnet, interlayer interaction

1. Introduction

In the two-dimensional (2D) Heisenberg model, it is well known that no spontaneous magnetization at any finite temperature can exist [1]. However another type of phase transition at a finite temperature seems not to be completely excluded until now. Early in the 2D Heisenberg model, Stanley and Kaplan's theory suggested a finite temperature divergence of susceptibility on the basis of high temperature series expansion [2], although further studies refuted the Stanley-Kaplan transition. Rigorous results show an exponential divergence of susceptibility at zero temperature [3]. After Stanley and Kaplan, some other possibilities of phase transition, including a glass phase [4], have been suggested [5], almost of which seems to be disproved [6]. Nevertheless, a weak anisotropy or a weak interlayer interaction has been known to allow a finite temperature transition in the 2D Heisenberg model [6, 7] and, recently, a Monte Carlo study of phase coherence in the 2D Heisenberg model suggested a fluctuationless coherent phase as in the 2D *XY* model below $k_BT_c/J \cong 0.46$ [8], where k_B and J are the Boltzmann constant and the exchange integral, respectively.

Contrasting to the 2D case, in the 3D Heisenberg model a finite temperature magnetic transition is evident at the critical coupling $K_c = J/(k_BT_c) = 0.69$ [9]. The accurate result for the 3D Heisenberg model gives an other chance to study the phase transition in the 2D case. In the 3D Heisenberg model interlayer interactions can be controlled (so called layered Heisenberg model) and in the limit of zero interlayer interaction the layered Heisenberg model corresponds to the 2D Heisenberg model. Phase transitions in the layered Heisenberg model have been studied by a renormalization group [7] and a spin wave theory [10]. An experimental measurement of transition temperature for the layered Heisenberg antiferromagnet with variable interlayer distances was reported, recently [11]. While the theoretical approaches show a logarithmic divergence of the critical coupling with decreasing interlayer interaction [10], which guarantees an absence of finite temperature phase transition in 2D case, the experimental measurement shows that the transition temperature leads to a finite value with increasing interlayer distance [11]. The experimental result contrasting to the theoretical one may be due to some additional interactions and anisotropies, as commonly does in real experiments. In this work, Monte Carlo method was employed to study the phase transition in the layered Heisenberg model with variable interlayer interactions.

2. Monte Carlo Simulation

The classical Heisenberg ferromagnet with variable interlayer interactions is described by the following model Hamiltonian with spin quantum number $S = 1$,

$$H = -J_{ij} \sum_{\langle ij \rangle} ((S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z), \qquad (1)$$

where the exchange integrals $J_{ij} = J$ for i, j being nearest neighbors in the same plane and $J_{ij} = J'$ for i, j in different planes. $J = J'$ corresponds to the three-dimensional Heisenberg case, and $J' = 0$ to the two-dimensional Heisenberg case.

Each spins are placed on an L^3 cubic lattice with $L = 10$. Periodic boundary conditions were applied to eliminate boundary effects. The traditional metropolis algorithm was employed to change the spin configuration. All the measurements were carried with decreasing temperature from

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an infinite temperature, *i.e.* from a completely disordered phase. In order for thermal equilibration, 2000-20000L^3 MCS's (Monte Carlo Step) depending on J/J' were consumed. Each measurement were taken at every $(L/2)^3$ MCS (L^3 MCS near the critical temperature) in order to avoid a correlation between the measurements. As a result, 20000-80000 averages for a physical quantity were carried.

The measured quantities are the spontaneous magnetization M and the susceptibility defined by

$$M = \frac{1}{L^3}\ \langle [(\Sigma \vec{S}_i)^2]^{1/2} \rangle,$$

$$x = \frac{1}{T}\left[\frac{1}{L^3}\langle (\Sigma \vec{S}_i)^2 \rangle - M^2\right],$$

where < ... > indicates an ensemble average. And the temperature of maximum susceptibility was adopted as a transition temperature.

3. Results and Discussion

Fig. 1 shows the spontaneous magnetization. Due to a finite size effect, a spontaneous magnetization is observed even in the paramagnetic phase and the phase transition is smoothed. Fig. 2 shows the measured susceptibility. The weaker the interlayer interaction becomes, the larger the maximum amplitude is, which in turn requires much longer time for thermal equilibration.

Fig. 3 shows the critical coupling, $K_c = J/T_c$, obtained from the temperature of maximum susceptibility as a function of $\ln(J/J')$. The critical coupling at $\ln(J/J') = 0$, corresponding to the 3D Heisenberg case, well coincides with the reported one, $K_c = 0.69$ [9]. Both a renormalization group [7] and a spin wave theory [10] have suggested a logarithmic dependence of critical coupling on J/J'. The linear fit in Fig. 3 evidently shows the logarithmic dependence.

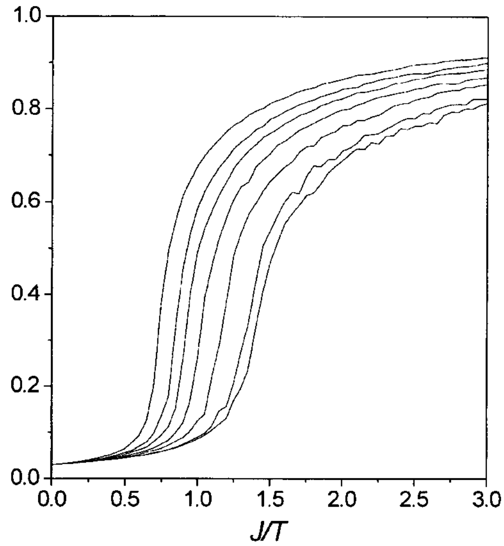

Fig. 1. Spontaneous magnetization vs J/T. From the left line, each line corresponds to $J/J' = 1$, 1.5, 2, 3, 5, 10, and 14.

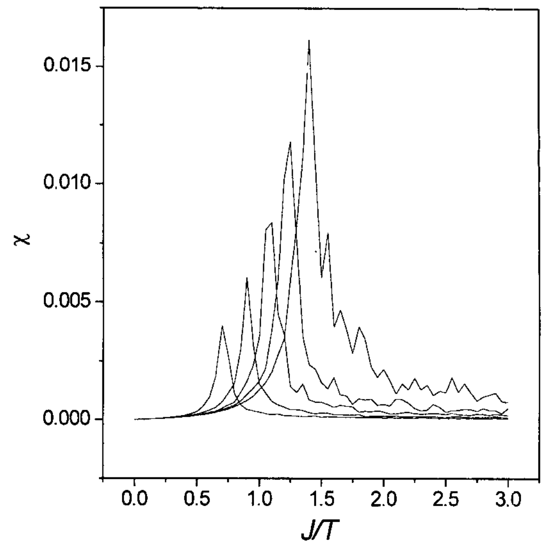

Fig. 2. Susceptibility vs J/T. For clarity, four lines corresponding to four different J/J' are shown.

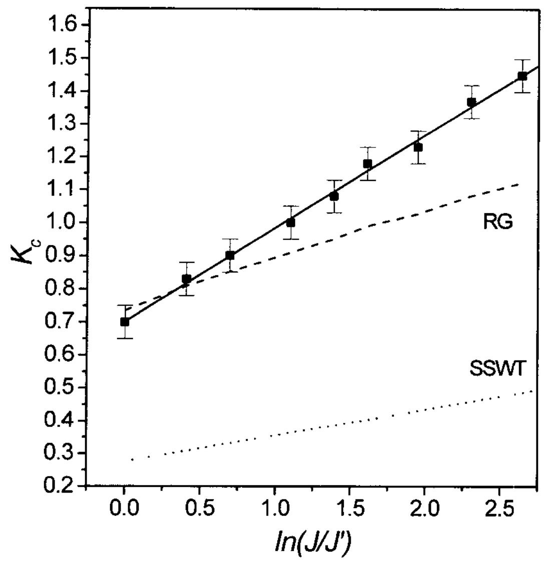

Fig. 3. Critical coupling $K_c = J/T_c$ vs $\ln(J/J')$. The solid line shows a linear fit corresponding to eq. (7). The dotted line corresponds to eq. (3), the self-consistent spin-wave theory (SSWT). The dashed line corresponds to eq. (5), the renormalization group theory (RG).

In a recent self-consistent spin-wave theory, the transition temperature in the layered Heisenberg magnet was described as follows, with $1 << J/J' << 2S$ [10],

$$T_c = \frac{4\pi J S^2}{\ln(32SJ/(J'\gamma_c'))}, \qquad (2)$$

where $\gamma_c' = T_M/(4\pi JS)$. In the classical limit, $\gamma_c'/S = 1$, Eq. (2) is further reduced to a simpler form as, with $S = 1$,

$$K_c = \frac{J}{T_c} = \frac{1}{4\pi}\left[\ln 32 + \ln\frac{J}{J'}\right]. \qquad (3)$$

The dotted line in Fig. 3 corresponds to Eq. (3), which lies far below the Monte Carlo results. As has been known, a spin-wave theory is correct in the low temperature region but becomes erroneous near the critical temperature [6].

A more correct description of the transition temperature is given by a renomalization group approach as follows [7],

$$t_c = 2/\left[\ln \frac{128}{a_r t_c} + 2 \ln \frac{1}{t_c} + \Phi\right], \tag{4}$$

where $t_c = T_c/(2\pi JS^2)$, $a_r^{-1} = (1-t_c/4)(J/J')$, and Φ is a contribution from non-spin-wave fluctuations. With $S = 1$ and neglecting Φ, Eq. (4) can be expressed as a form of critical coupling,

$$K_c = \frac{1}{4\pi}\left[\ln 128 + 3 \ln (2\pi K_c) + \ln\left(1 - \frac{1}{8\pi K_c}\right) + \ln \frac{J}{J'}\right]. \tag{5}$$

The dashed line in Fig. 3 corresponds to Eq. (5), which is much closer to the Monte Carlo results than that of the self-consistent spin-wave theory, particularly around the 3D case. But the renormalization group approach shows an increasing discrepancy from our Monte carlo results with decreasing interlayer interaction.

An easy explanation of the logarithmic dependence comes from the vortex excitations as in the XY model [12]. A characteristic length $R_1 = a(J/J')^{1/2}$ of the 3D vortex ring in each layer has to be compared with the correlation length $R_c = a\exp(2\pi J/T)$ in the 2D Heisenberg magnet. When $R_1 = R_c$, the interlayer interaction favours a spontaneous magnetization. Then the transition temperature can be estimated as:

$$T_c = 4\pi J/\ln(J/J'). \tag{6}$$

Eqs. (2) and (6) coincide with each other except for a factor of 32. The logarithmic dependence is originated from the exponential divergence of the correlation length. The coefficient $1/4\pi$ of $\ln(J/J')$, common in Eqs. (3), (5), and (6), should be replaced by $0.3 \simeq 1/\pi$ in our empirical formula for the critical coupling as follows,

$$K_c = 0.7(\pm 0.01) + 0.3(\pm 0.03)\ \ln(J/J'). \tag{7}$$

which is obtained from the linear fit in Fig. 3. The tolerances are simply the fitting errors. Because the coefficient $1/4\pi$ is related to the characteristic size of vortex, the observed discrepancy between the theoretical expectation and our Monte carlo results seems to be due to a misestimation of the characteristic size.

In summary, we have studied the phase transitions in the layered Heisenberg magnet by means of Monte Carlo simulation. The critical couplings obtained from the simulation show a strong logarithmic dependence on J/J' and fairly differ from the theoretical expectations. In additon, an empirical formula for the critical coupling was obtained.

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