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Abstract. A three-dimensional array of classical XY spins with couplings $J_{\parallel}$ in the planes and $J_{\perp}$ between planes is studied both analytically and numerically. For an infinite number of planes, the magnetization is shown to be extremely sensitive to the interplane coupling. For a finite number N of planes, the magnetization vanishes, but there is a (Kosterlitz-Thouless) transition. The critical temperature increases as a function of N and rapidly approaches the bulk value.

Introduction

It is well established that the two-dimensional XY model undergoes a phase transition of a particular type, as described first by Berezinskii and by Kosterlitz and Thouless [1]. According to Mermin-Wagner theorem, below the critical temperature the order parameter remains zero, while the susceptibility is infinite. Here we consider a collection of coupled XY planes defined by the Hamiltonian

$$H = -J_{\parallel} \sum_{\ell} \sum_{<ij>} \vec{s}_{i\ell} \cdot \vec{s}_{j\ell} - J_{\perp} \sum_{\ell i} \vec{s}_{i\ell} \cdot \vec{s}_{i\ \ell+1} \tag{1}$$

where $\vec{s}_{i\ell}$ is a unit vector on site i in the ℓ'th plane. We find that any small interplane coupling, $J_{\perp} \ll J_{\parallel}$, changes the nature of the transition [2].

Order Parameter for an Infinite Number of Planes

At low temperatures we can use the spin wave approximation for the magnetization, giving

$$m = \exp\left(-\frac{k_B T}{2J_{\parallel}}\alpha\right) , \tag{2}$$

where

$$\alpha = \frac{1}{(2\pi)^3} \int_{BZ} d^3q \ \frac{J_{\parallel}}{\omega(\vec{q})} \tag{3}$$

and the spin wave spectrum is

$$\omega(\vec{q}) = 4J_{\parallel} \left[\sin^2 \frac{q_x}{2} + \sin^2 \frac{q_y}{2}\right] + 4J_{\perp} \sin^2 \frac{q_z}{2}. \tag{4}$$

For $J_{\perp} \rightarrow 0$, the parameter α diverges logarithmically and the magnetization tends to zero. This is in agreement with the upper bound

$$m \leq \left(\frac{J_{\parallel}}{k_B T \alpha}\right)^{1/2} , \tag{5}$$

derived as a straightforward generalization of the Mermin - Wagner theorem [3]. Fig. 1 shows that an extremely small $J_{\perp}$ is sufficient to efficiently suppress the fluctuations, thus stabilizing the long-range order.

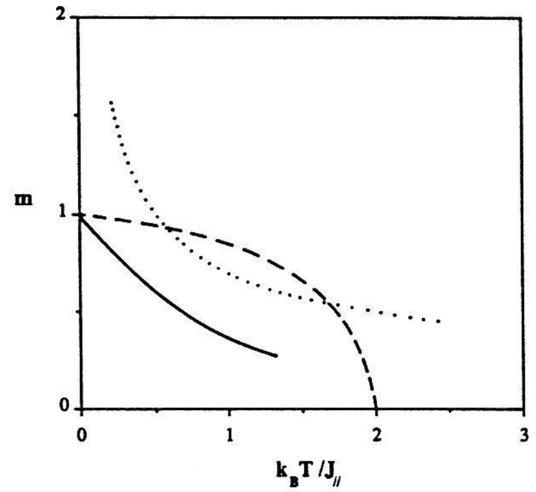

Figure 1 : Order parameter for an infinite number of planes and a ratio $J_\perp/J_\parallel = 10^{-10}$. The dashed line represents the mean-field approximation, the solid line Eq. (2) and the dotted line the r.h.s. of Eq. (5).

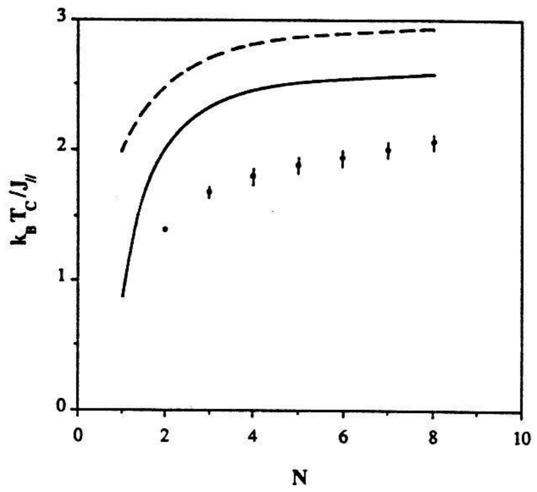

Figure 2 : Critical temperature for a finite number of planes in the isotropic case, $J_\perp = J_\parallel$. The dashed-line represents the mean field result, the full line Eq. (6) and the dots the Monte Carlo simulations.

Critical Temperature for a Finite Number of Planes

It is easy to show that for any finite number N of planes the magnetization vanishes for $T > 0$. In order to estimate the critical temperature T_c where the susceptibility diverges we treat the coupling between planes in a mean-field approximation and find the implicit relation

$$1 = 2J_\perp \cos\left(\frac{\pi}{N+1}\right)\chi_{2D}(T_c). \tag{6}$$

Here $\chi_{2D}(T)$ is the susceptibility of the two-dimensional XY model for which we use the high-temperature expansion of Butera et al. [4]. We have also performed Monte Carlo calculations, using a cluster algorithm and a reweighting procedure. The critical temperature was determined on the basis of the fourth cumulant of the magnetization. The results are shown in Fig. 2 for the isotropic case, $J_\perp = J_\parallel$. We see that T_c first increases rapidly as a function of N and then approaches the limiting value for the 3D XY model. For smaller values of $J_\perp$ the overall increase of T_c is smaller. The comparison between the results based on Eq. (6) and the Monte Carlo data indicates that inter-plane fluctuations considerably reduce the critical temperature.

References

[1] For a review see, e.g., P. Minnhagen, Rev. Mod. Phys. 59, 1001 (1987).

[2] A more detailed description of our results will be given elsewhere.

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

[4] P. Butera, M. Comi and G. Marchesini, Phys. Rev. B 40, 534 (1989).