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Kosterlitz-Thouless transition in a two-dimensional isotropic antiferromagnet in a uniform field

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The transition temperature in the classical two-dimensional isotropic antiferromagnet in a uniform magnetic field, applied perpendicular to the *xy* plane, is calculated using a self-consistent spin-wave theory. The effect of vortex-antivortex bound pairs to the transition temperature is estimated.

It is now well known[1,2] that the two-dimensional classical XY model undergoes a vortex-unbinding transition in a narrow temperature region in which vortex bound together in pairs unbind. For temperatures low enough, all vortices are bound together in pairs and the unbinding transition starts at a critical temperature T_{KT} at which the model undergoes a thermodynamic phase transition, the Kosterlitz-Thouless (KT) transition. On the other hand the isotropic Heisenberg model is believed to have no phase transition and it is also believed that its magnetic susceptibility diverges strongly as the temperature approaches zero.[3] However, a two-dimensional classical isotropic Heisenberg antiferromagnet in a uniform magnetic field applied perpendicular to the xy plane is expected to have the XY-like low-temperature phase and show the KT transition due to a XY-like degeneracy of a canted spin-flop ground state.[4] Using Monte Carlo simulations Landau and Binder[5] have studied the phase boundary between the spin-flop phase and the paramagnetic phase for this model. Their simulations indicate that the KT transition temperature approaches zero extremely slowly as the field approaches zero. In this paper we calculate the transition temperature for this model using a self-consistent harmonic theory, developed before to study the anisotropic Heisenberg model.[6] We will start with the following Hamiltonian

$$H=\frac{J}{2}\sum_{r,a}\mathbf{S}_r\cdot\mathbf{S}_{r+a}-H\sum_r S_r^z , \tag{1}$$

where $\mathbf{S}_r$ is a classical spin (we take $S=1$) and $r+a$ labels the nearest-neighbor sites of r (the sum runs over all pairs of nearest-neighbor spins on the square lattice). At zero temperature the spin-flop ground state has the following polar angles:[5] $\phi_0=0$, $\theta_0=\cos^{-1}(H/8J)$, and the spin-flop–to–paramagnetic transition occurs at a critical field $H_c=8$ J.

In order to treat the magnetic field term in a proper way, we will first introduce the parametrization[7]

$$\mathbf{S}_n=(-1)^n\{\sin[\theta_n+(-1)^n\theta_o]\cos\phi_n,\sin[\theta_n+(-1)^n\theta_o]\sin\phi_n ,\cos[\theta_n+(-1)^n\theta_o]\} , \tag{2}$$

where the even n describes one sublattice, the odd n the other one. Taking Eq. (2) into Eq. (1) we find that keeping only terms of second order the Hamiltonian becomes

$$H=\tfrac{1}{4}\sin^2\theta_o\sum_{r,a}(\phi_r-\phi_{r+a})^2-2J\sum_r(\theta_r-\theta_o)^2 -\frac{J}{2}\sum_{r,a}(\theta_r-\theta_o)(\theta_{r+a}-\theta_o)+\frac{H}{2}\cos\theta_o\sum_r(\theta_r-\theta_o)^2 . \tag{3}$$

Redefining the spin component S^z by

$$S_r^z=\cos(\theta_r-\theta_o) ,$$

we see that, from the thermodynamical point of view, our original model is equivalent to an anisotropic ferromagnet described by the Hamiltonian

$$H=-\frac{J}{2}\sum_{r,a}[\sin^2\theta_o(S_r^xS_{r+a}^x+S_r^yS_{r+a}^y)+S_r^zS_{r+a}^z] +A\sum_r(S_r^z)^2 \tag{4}$$

with $A=H^2/8J$.

Now, in order to use the self-consistent approximation, we write Hamiltonian (4) in terms of the polar representation for the spin at site r

$$\mathbf{S}_r=\{[1-(S_r^z)^2]^{1/2}\cos\phi_r,[1-(S_r^z)^2]^{1/2}\sin\phi_r,S_r^z\} . \tag{5}$$

Following the same procedure used in Ref. 6 we obtain the following quadratic form of Hamiltonian (5)

$$H_o=\frac{J}{2}\sum_q\{\rho(1-\gamma_q)\phi_q\phi_{-q}+[(1-\gamma_q)+2A/J]S_q^zS_{-q}^z\} , \tag{6}$$

where $\gamma_q=\frac{1}{2}(\cos q_x+\cos q_y)$, and the spin-stiffness constant is given by

$$\rho=\sin^2\theta_o\langle[1-(S_r^z)^2]^{1/2}[1-(S_{r+a}^z)^2]^{1/2} \times\cos(\phi_{r+a}-\phi_r)\rangle . \tag{7}$$

The stiffness takes into account anharmonic terms neglected when we write the original Hamiltonian in the harmonic form. Following Ref. 6 we find that we can write Eq. (7) as

$$\rho=\sin^2\theta_o[1-tI(H)]\exp(-t/\rho)\ , \tag{8}$$

where $t=T/4J$ and

$$I(H)=\frac{1}{(2\pi)^2}\int\frac{dq}{1-\gamma_q+H^2/4J}\ . \tag{9}$$

Equation (8) is a self-consistent equation giving the stiffness ρ for each temperature. The anharmonicity of the original Hamiltonian (4) results in a abrupt disappearance of the stiffness, indicating a phase transition, at a temperature T_c given by

$$T_c(H)=4J\sin^2\theta_o[e+\sin^2\theta_o I(H)]^{-1}\ . \tag{10}$$

Near the critical field $I(H)$ is small and Eq. (10) reduces to

$$T_c(H)=T_{KT}[1-(H/8J)^2]\ , \tag{11}$$

where $T_{KT}=4J/e$ is the critical temperature of the plane rotator model.[1] Equation (11) agrees with the one obtained by Landau and Binder[5] using first-order spin wave theory. In this limit expression (11) is expected to be correct because near H_c the fluctuations of S_r^z are suppressed at low temperatures.

Our theory is also expected to work better for small magnetic fields. In the region $H \ll H_c$, Eq. (9) gives

$$I(H)\approx\frac{2}{\pi}\ln\left[\frac{4\pi J^2}{H^2}\right] \tag{12}$$

leading to

$$T_c(H)\approx\frac{4J}{e+(2/\pi)\ln(4\pi J^2/H^2)}\ . \tag{13}$$

For very small magnetic fields we obtain from Eq. (13)

$$T_c(H)\approx 2\pi J/\ln(4\pi J^2/H^2)$$

in agreement with a result predicted by Okwamoto,[4] who estimated the transition temperature for Hamiltonian (1) by calculating the instability temperature at which the free-energy vanishes, in the limit where a vortex pair changes into an instanton.

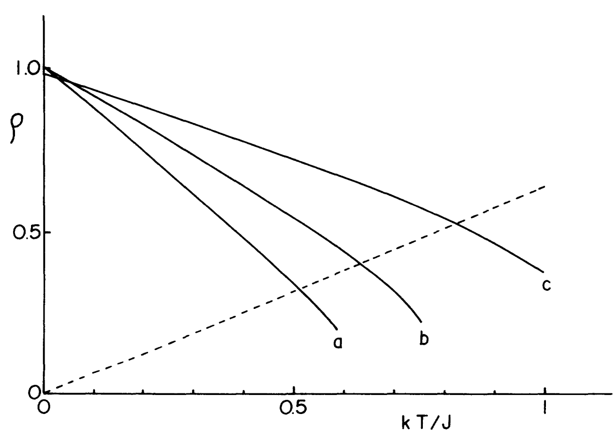

FIG. 1. Temperature dependence of the stiffness for (a) $H=0.01$, (b) $H=0.1$, and (c) $H=1.0$. The dotted line corresponds to $\gamma=(2/\pi)T$. The critical temperature occurs at the point of intersection of $\rho(T)$ and $(2/\pi)T$.

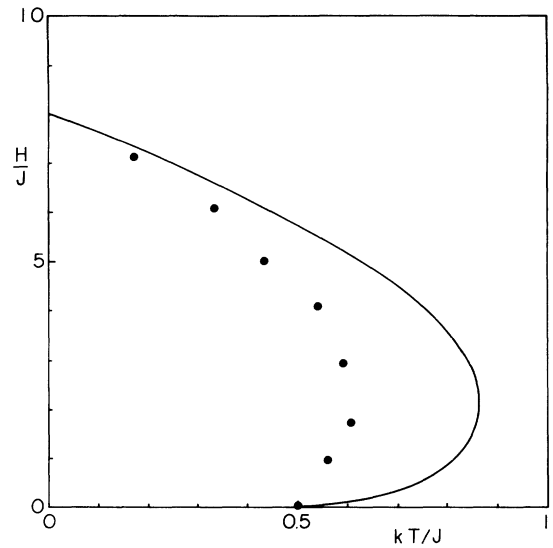

FIG. 2. Phase boundary for the isotropic Heisenberg antiferromagnet in a uniform magnetic field. The solid line represents our theoretical calculation. The solid circles are data obtained from Monte Carlo simulation for fields between $H/J=0.01$ and 7.0 by Landau and Binder.

The stiffness ρ calculated using the self-consistent technique does not incorporate the effect of polarization by bound vortex pairs.[8] This latter mechanism is responsible by a shift in the Kosterlitz-Thouless transition temperature.[2] At T_{KT} renormalization-group analysis[9] shows that the stiffness should exhibit a universal jump given by $2T_{KT}/\pi$. The Kosterlitz-Thouless temperature for our model can then be determined by the crossing between the $\rho(T)$ curve, calculating using Eq. (8) and the line $\gamma=2T/\pi$. In Fig. 1 we plot both curves for some values of H. The transition temperature, calculated using this approach, is shown in Fig. 2 as a function of the magnetic field, where we compare our calculation with data obtained from Monte Carlo (MC) simulations performed by Landau and Binder.[5] For $H/J=0.01$ (the

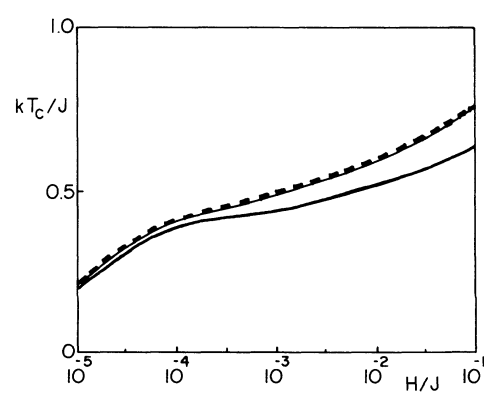

FIG. 3. Transition temperature as a function of the field H. The dashed line represents the calculation given by Eq. (10). The solid line represents the calculation as described in Fig. 1.

lowest field where data was available) we obtained $T_c/J=0.51$ in good agreement with the value of T_c obtained in MC simulations. In Fig. 3 we show T_c, as a function of H, for realistic values (from the experimental point of view) of the magnetic field H. In this figure we show T_c calculated using Eq. (10) and T_c calculated using the technique described in Fig. 1. As we can see, the transition temperature approaches zero very slowly as the field approaches zero. In addition, the fact that the out-of-plane fluctuations have an important effect on the calculation of the transition temperature should be stressed.

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