Magnetization: A characteristic of the Kosterlitz-Thouless-Berezinskii transition

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In the low-temperature phase of the two-dimensional XY model, spin-spin correlations decay so slowly with distance that the thermodynamic limit is inaccessible. As a result the Mermin-Wagner theorem is inapplicable to any realizable system, and all have a measurable finite-size magnetization. We show that there is a regime of universal behavior near to the Kosterlitz-Thouless-Berezinskii transition. In experiments, the regime is identified by a magnetization exponent $\beta=0.23$, which we have calculated by a renormalization-group analysis. Monte Carlo simulations of an harmonic XY model clearly locate the boundaries of the universal regime, and identify it with vortex renormalization.

Twenty years after the original papers of Kosterlitz and Thouless and Berezinskii[1] it is still a subject of debate as to whether "KT theory" is a truly accurate description of the two-dimensional XY (2D XY) magnet.[2] Verification of the theory—whether by numerical simulation, series expansion, or experiment on real magnets—is made problematic by the lack of an easily measurable and definitive characteristic of the KTB transition.[3] In a recent calculation[4] we have shown that such a characteristic exists, and that ironically it is a magnetization. There is, of course, no magnetization in the *infinite* 2D XY model,[5] but as originally pointed out by Berezinskii and Blank,[6] even a macroscopic 2D XY model has a measurable finite-size-induced magnetization. We used this fact to explain the apparently universal magnetic exponent $\beta=0.23$,[4,7] observed in all experiments on materials which approximate the model, such as layered magnets and the recently developed ultrathin magnetic films.[8] The latter are of particular interest as they are truly two dimensional.

In Ref. 4 we showed that $\beta=0.23$ is observed in Monte Carlo simulation, and can be calculated from the standard renormalization-group (RG) analysis[9,10] of the 2D XY model. We did not explore the more fundamental question of why scaling behavior should occur in a finite system. In this paper we examine the physical content of our finite-size scaling analysis by means of Monte Carlo simulation of an harmonic 2D XY model. We show that the model has several well-defined regimes, with sharp and distinct crossovers between them. One of these, the vortex renormalized spin-wave regime, is characterized by a separation of the important length scales, allowing the approach towards scaling behavior. Our results confirm the accuracy of KT theory in this region.

The XY Hamiltonian is

$$H=-J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j=-J\sum_{\langle i,j\rangle}\cos(\theta_i-\theta_j)\ , \qquad (1)$$

where J is the coupling constant, $\mathbf{S}_i$ is a 2D classical spin vector of unit length at site i, and θ_i is an angle of rotation within the spin plane. If the cosine function in (2) is expanded, and only the quadratic term is retained, the magnetization can be calculated exactly at all temperatures. The result is[6,11]

$$M(N,T)=\left\langle\left|\frac{1}{N}\sum_{i=1,N}\mathbf{S}_i\right|\right\rangle=\left[\frac{1}{2N}\right]^{1/8\pi K}\ , \qquad (2)$$

where the angular brackets represent a thermal average and $K=1/T$ is the spin-wave stiffness (temperature is in units of J/k_B throughout). One can get an order-of-magnitude estimate of the effects of finite size[4] by putting the "mean-field" transition temperature[1] $T_{\mathrm{KT}}\approx\pi/2$ into Eq. (2). With $M(N,T_{\mathrm{KT}})\lesssim 0.01$ as a reasonable estimate for the thermodynamic limit, the sample would need to be bigger than the state of Texas for the Mermin-Wagner theorem to be relevant!

The harmonic XY (HXY) model again retains only the quadratic term in the expansion of the cosine function in (2), but also maintains the periodicity of the original cosine interaction in the partition function. The spins interact via the potential

$$H=-J[1-\tfrac{1}{2}(\theta_i-\theta_j-2\pi n)^2]\ , \qquad (3)$$

where n is an integer ensuring that $(\theta_i-\theta_j-2\pi n)$ is bounded between $\pm\pi$. This approximation corresponds closely to the system of noninteracting spin waves and vortex pairs studied in KT theory.[12] The vortices can be mapped onto a neutral charge system,[1] and are simultaneously referred to as a 2D Coulomb gas. Numerical results for the HXY model should correspond closely to the predictions of RG calculations, and any deviation of the magnetization from the harmonic spin-wave expression (2) can only be due to vortices.

We have performed Monte Carlo simulations of the magnetization of the HXY model for systems of 10^2, 10^3, and 10^4 spins. The results for the largest system are shown in Fig. 1, with the XY data of Ref. 4 included for comparison. The results are an average of three to nine simulations each with 10^5 Monte Carlo steps per particle per temperature.

The dashed line shows the exact spin-wave result of Eq. (2). The HXY data are fitted extremely well by (2) for

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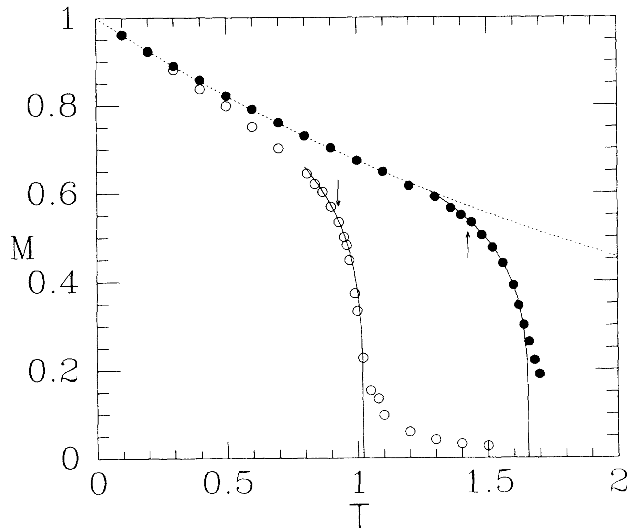

FIG. 1. Magnetization vs temperature for a Monte Carlo simulation of a system of $N=10^4$ spins, for the HXY model (solid circles) and 2D XY model (open circles). The solid curves show, in each case, the fit to scaling behavior, with exponent $3\pi^2/128$ (see text). The dashed curve is the spin-wave result of Eq. (2). The arrows mark T^*, with "up" arrow for the HXY model and a "down" arrow for the 2D XY model. We find $T_C^{HXY}=1.655$, $T^*_{HXY}=1.427$, $T_C^{XY}=1.020$, $T^*_{XY}=0.928$.

all temperatures $T/T_{KT} \lesssim 0.96$, where $T_{KT}=1.351$.[13] This indicates that the density of thermally excited vortex pairs is negligible up to a temperature close to T_{KT}. Above this temperature the magnetization suddenly deviates from Eq. (2), indicating the thermal excitation of vortices. The data in this region are accurately described by a power law, as shown in Fig. 1. Free fits of a power law to the data, between $T=1.3$ and 1.6 give an exponent $\beta=0.23\pm0.01$. The accuracy of the free fits increases with system size, with the errors being noticeable for 10^2 spins. These are at first sight very surprising results, but they are in agreement with simulations on the XY model, and experimental results on all known XY-like layered magnets and thin films.[4,7] The common denominator of all these observations is that the power-law behavior with $\beta=0.23$ is not observed asymptotically at the point where the magnetization approaches zero, T_C. Instead, it occurs over a finite range of temperature close to, but *below*, T_C. This distinguishes β from a conventional critical exponent. Empirically, the magnetization may be written $M(T\to T^*)\sim(T-T_C)^{0.23}$, where T^* is a temperature near T_{KT} at which the power-law behavior best holds.

In Ref. 4, we showed that KT theory, when applied to a finite system, naturally predicts this behavior, and forces on us precise definitions of the two temperatures T^* and T_C. The solid lines in Fig. 1, in fact, represent the theoretical predictions of our previous work,[4] these being *coincident* with the best free power-law fits.

In the RG treatment[9,10] of the infinite system the vortex excitations are irrelevant below T_{KT} and are renormalized into an effective spin-wave stiffness K_{eff}. At T_{KT} the vortices unbind, and K_{eff} jumps discontinuously to zero from the universal value $K_{eff}(T_{KT})=2/\pi$. We obtain an approximate expression for the magnetization, in the presence of vortex pairs, by replacing K with K_{eff} in Eq. (2). Hence we have a magnetization for all $K_{eff}>0$. In a finite-sized system, however, K_{eff} does not drop discontinuously to zero at T_{KT}. Rather the termination of the renormalization flow at a length scale equal to L, the system size, rounds out the universal jump, and both the spin-wave stiffness and the magnetization fall steeply, yet continuously to zero.

The RG equations are linearized about the fixed point $K_{eff}=2/\pi$. Physically this fixed point corresponds to scaling behavior of the Coulomb gas of vortices. Changing the length scale removes all vortex pairs on lengths less than the new scale parameter, however, fixed point behavior is such that the vortex pair distribution remains unchanged. For a given temperature $T\gtrsim T_{KT}$ two lengths arise naturally in the calculation. The first, L^*, is the value of the rescaling parameter b giving $K_{eff}=2/\pi$. The second, $L_C\approx(L^*)^2$, is the value of b where the linearized equation break down, and K_{eff} diverges from the fixed point. For $T\gtrsim T_{KT}$ one has $1\ll L^*\ll L_C$, where L^* and L_C are expressed in units of the lattice constant. This separation of length scales allows the identification of two well-defined regimes. For $b\approx L^*$, K_{eff} renormalizes extremely slowly with length, and the system approaches fixed point behavior with Coulomb gas scaling of the vortices. In this regime the power-law behavior of the spin-spin correlation function is maintained. In the second regime, with $b\gtrsim L_C$, the vortex pair distribution renormalizes rapidly to that of a gas of free vortices, which results in K_{eff} renormalizing towards zero, and the development of exponentially decaying spin correlations. Putting the correlation length ξ equal to L_C yields the Kosterlitz expression[9] for ξ, which diverges exponentially with $\sqrt{T-T_{KT}}$.

For fixed system size, $L=\sqrt{N}$, the same analysis yields two characteristic temperatures. The first, $T^*(L)$ is the temperature at which $K_{eff}=2/\pi$, and the second, $T_C(L)$, is the temperature at which the spin-spin correlation length ξ equals the system size. We interpret $T_C(L)$ as the effective Curie temperature for the finite-sized system. $T^*(L)$ and $T_C(L)$ are both shifted logarithmically from T_{KT} with size L giving[4,14]

$$T_C(L)-T_{KT}=4[T^*(L)-T_{KT}]=\frac{\pi^2}{c(\ln L)^2}\ , \qquad (4)$$

The logarithmic dependence on L, as opposed to a power law, is a standard result of finite-size scaling in the 2D XY model.[15] It ensures that, for fixed L, the range of temperature, $\sim T_C-T^*$, over which scaling behavior occurs is unusually large. This explains the experimental and numerical observation that apparent critical behavior is measured at temperatures well below T_C.

The separation of length scales and the asymptotic approach to fixed point behavior is illustrated in Fig. 2, where K_{eff}, as given by the linearized RG equations, is plotted as a function of scale parameter b [from Eq. (4) of Ref. 4]. The RG equations are strictly valid only in the limit of very large system size, and b relates K_{eff} for different size ratios. An assumption of our calculation is

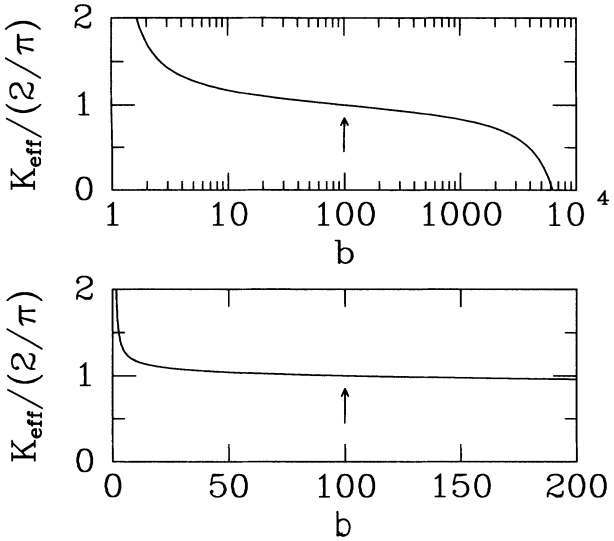

FIG. 2. Renormalized spin-wave stiffness $K_{eff}/(2/\pi)$ vs scale parameter b, as given by the linearized RG theory with $c=1.51$ (Ref. 16). The arrows mark $b=L^*$.

that $b\sim O(1)$ can be identified with a microscopic length scale. In Fig. 2, the temperature is fixed at a value corresponding to T^* for a system size $L=100$. In the upper curve, with b on a logarithmic scale, three regimes of behavior are visible. It is the intermediate regime, with K_{eff} approximately constant, illustrated in the lower curve, that results in asymptotic fixed point behavior.

Numerically we find that the constant c decreases, with system size,[16] below the initial estimate of Kosterlitz, $c\approx 2.1$.[9] The existence of a finite value for c has implications for the ultimate validity of KT theory, in the thermodynamic limit. Our data show that, with these determined values of c, KT theory is at least asymptotically correct for the large, but finite systems that exist in nature.

After replacing K with K_{eff} in Eq. (2) we define the magnetization exponent β as the tangent to the curve of $\ln M(L,T)$ against $\ln[t(L)]$, where $t=T_C-T$. At $t^*=T_C-T^*$, we find[4] $\beta(L,T^*)=3\pi^2/128=0.231\ldots$. The validity of the calculation rests on K_{eff} varying very slowly with wavelength, which is the case at T^* (see Fig. 2).

T^* may in this sense be regarded as a universal point, where the magnetization scales with system size, field H and temperature. The universal properties of the finite system at T^* may be summarized[4]

$$K_{eff}(L)=2/\pi\ , \tag{5}$$

$$\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle_{r<L}\sim r^{-1/4}\ , \tag{6}$$

$$M(L,T\to T^*)=B(T_C-T)^{3\pi^2/128}\ , \tag{7}$$

$$M(L,T^*)=\left[\frac{1}{\sqrt{2}L}\right]^{1/8}\ , \tag{8}$$

$$M(H,L,T^*)-M(0,L,T^*)\sim H^{1/15}\ , \tag{9}$$

where $\langle \mathbf{S}_0\cdot\mathbf{S}_r\rangle$ is the spin-spin correlation function, with distance r, and B is a size dependent amplitude, defined by equating (7) and (8) at T^*. At T_C, in contrast, the finite system has the properties $K_{eff}(L)\to 0$, $M(L)\to 0$, $\xi=L$. In the infinite system these two temperatures coincide with T_{KT} giving the universal jump in K_{eff}.

Our interpretation of the two temperatures T^* and T_C is confirmed by the Monte Carlo "snapshots" shown in Fig. 3. At T^* [Fig. 3(a)] the spin waves coexist with a low density of vortices which appear to be in well-defined pairs, as assumed in KT theory.[9] At this temperature, unbound vortices should only be evident on a length scale L_C, orders of magnitude greater than the system size L. At T_C, however, $L=L_C$, and unbound vortices are ex-

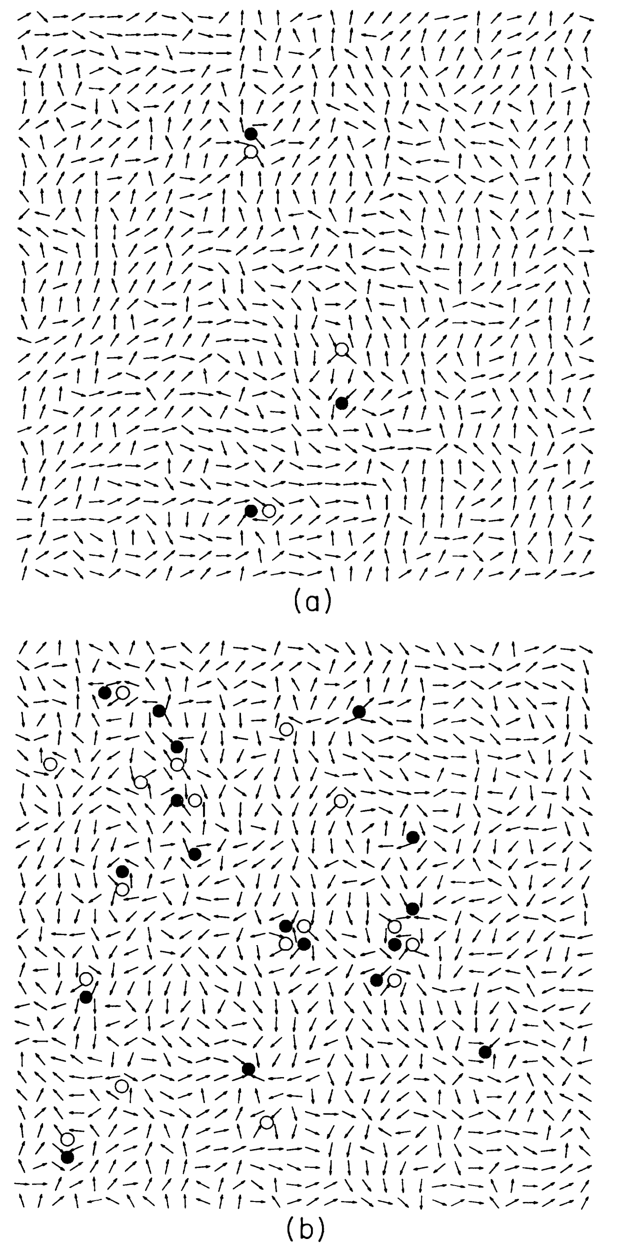

FIG. 3. Monte Carlo "snapshots" showing spin and vortex configuration for the HXY model, with $N=1024$, at T^* (a) and T_C (b). The vortex positions are calculated by summing $\theta_i-\theta_{i+1}$ (Refs. 11 and 17) around each square plaquette of the lattice. Solid (open) circles represent positive (negative) vortices centered on plaquettes with a circulation of $+(-)2\pi$.

pected in nearly all snapshots. This is confirmed by Fig. 3(b), where there is clear evidence of vortex unbinding.

Comparing the data in Fig. 1 for the XY and HXY models, it is clear that the inclusion of the anharmonic corrections in the cosine interaction has the effect of reducing the vortex pair fugacity, hence reducing both the temperature scale over which scaling behavior takes place, and the absolute value of T_{KT}.[13] The anharmonicity causes the magnetization to fall below that of the linear spin-wave curve at relatively low temperature, even in the absence of vortex pairs.[17]

These results may be used to explain the behavior of ultrathin magnetic films.[8] We consider the most relevant case of a ferromagnetic film with a square or triangular lattice of magnetic atoms, in which the spins lie within the plane.[7] In such a system, any weak in-plane anisotropy will be fourfold or sixfold, and neither perturbation is strongly relevant.[4,10,18] The number of layers n is also irrelevant so long as n is small [that is $n \sim O(1)$],[19] and the dipolar coupling is only manifest on macroscopic length scales, where it causes domain formation. The 2D XY universality class is therefore robust to the dominant perturbations in the system, and one would expect to see 2D XY behavior over most of the temperature-field phase diagram. The ultrathin film is truly an anisotropic Heisenberg, rather than an XY system, and the presence of out-of-plane fluctuations would be expected to renormalize the temperature scale, and to reduce T_{KT} from the value expected for the XY model.[20] The finite size of the XY film may be the actual sample size, the average dipolar domain size, or a coherence length limited by defects. Its cause is not important, but its effect is to remove the long-wavelength spin waves which are responsible for the destruction of long-range order in the infinite system. As in the XY simulation (Fig. 1), with increasing temperature, the system should pass through four regimes: a linear spin-wave regime, an anharmonic spin-wave regime, a Coulomb gas scaling regime with $\beta \approx 0.23$, and finally a regime of finite-sized rounding. From the present work we conclude that only the Coulomb gas scaling regime is universal.

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[16] These fits have an adjustable parameter, the constant c. We find $c^{XY}_{1024} = 3.73$, $c^{XY}_{10^4} = 3.30$, $c^{HXY}_{10^2} = 2.0 \pm 0.3$, $c^{HXY}_{10^3} = 1.87$, $c^{HXY}_{10^4} = 1.51$, where the superscripts indicate the model and the subscripts the system size N. Other available estimates are $c^{XY} = 3.53$ (Ref. 2), $c^{\text{Villain}} \approx 2.1$ (Ref. 9), or ≈ 1.3 [W. Janke and K. Nather, Phys. Lett. A **157**, 11 (1991)].

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