Magnetization and universal sub-critical behaviour in two-dimensional XY magnets

1993 J. Phys.: Condens. Matter 5 L53

(http://iopscience.iop.org/0953-8984/5/4/004)

J. Phys.: Condens. Matter 5 (1993) L53–L59. Printed in the UK

LETTER TO THE EDITOR

Magnetization and universal sub-critical behaviour in two-dimensional XY magnets

S T Bramwell† and P C W Holdsworth‡

† Institut Laue–Langevin, 156-X, 38042 Grenoble, France

‡ Laboratoire de Physique, Ecole Normale Supérieure de Lyon, 69634 Lyon, France

Received 20 November 1992

Abstract. Layered magnets, considered to be experimental realizations of the 2D XY model, have a magnetization with a characteristic exponent $\beta = 0.23$. We show, using modified renormalization group equations, that this value of β is a universal signature of finite-sized 2D XY behaviour. We present simulation data in agreement with both the calculation and the experimental observations.

The two-dimensional XY model has long presented an interesting problem to both theoreticians [1] and experimentalists [2–8]. In the thermodynamic limit, at finite temperatures and in zero magnetic field the model cannot sustain long-range order [9], but nevertheless exhibits a 'Kosterlitz–Thouless–Berezinskii' phase transition [10] involving the unbinding of spin vortices at a critical temperature T_{KT}. In the low-temperature phase of bound vortices the correlation length remains infinite and the magnetization zero, as a result of the excitation of long-wavelength spin waves. The critical exponents η and δ vary continuously with temperature [11], but the exponents β, γ and ν are undefined.

Layered Heisenberg magnets with planar anisotropy can be treated as quasi-2D XY systems [12]. In these materials the spontaneous magnetization is stabilized by weak 3D coupling J' which determines the asymptotic critical behaviour. However at lower temperature there is a very sharp crossover to a second regime, which we refer to as 'sub-critical'. The magnetization exponents β measured in this range are listed in table 1. The compounds $BaNi_2(PO_4)_2$, Rb_2CrCl_4 and K_2CuF_4 are the best approximations to the ideal and represent a variety of lattice types, spin values and degrees of planar anisotropy. All have a well defined $\beta = 0.23$. The other compounds in the list have β varying between $\simeq 0.18$ and $\simeq 0.26$ [13].

Using modified renormalization group (RG) equations, we show that the magnetization of an arbitrarily large, but finite, 2D XY model approaches power-law behaviour over a restricted temperature range, with an effective exponent $\beta = 0.23$. This is a universal property of the 2D XY model and can be regarded, when observed in experiment, as a signature of 2D XY behaviour. We present Monte Carlo simulations in agreement with our calculation, and finally discuss the relationship between the calculation, and the experimental results of table 1.

Although there is no broken symmetry in the 2D XY model [9] the spin–spin correlation function has power-law decay at low temperature. This slow decay with

Table 1. Critical exponents β and the corresponding range of reduced temperature $(1-T/T_C)$, measured for 2D *XY* systems [12] (F = ferromagnet, A = antiferromagnet, Fo = (HCO_2), Ur = $(CO(NH_2)_2)$).

Compound	Type	β	Range	Reference
$BaNi_2(PO_4)_2$	A	0.23	0.02–0.4	[2]
K_2CuF_4	F	0.22	0.02–0.3	[4]
Rb_2CrCl_4	F	0.23	0.03–> 0.15	[7]
Gd_2CuO_4	A	0.23	0.02–0.3	[25]
$Rb_2CrCl_2Br_2$	F	0.26	0.04–0.8	[26]
Rb_2CrCl_3Br	F	0.26	0.03–0.9	[26]
$CoCl_2 \cdot 6H_2O$	A	0.18	0.04–0.4	[3]
Rb_2FeF_4	A	0.2	0.03–0.3	[3]
$CuFo_2 \cdot 4H_2O$	A	0.22	0.06–0.3	[27, 13]
$CuFo_2 \cdot 2Ur \cdot 2H_2O$	A	0.22	0.01–0.5	[27, 13]
$MnFo_2 \cdot 2H_2O$	A	0.23	0.015–0.5	[3, 13]

distance ensures a magnetization in a finite system [14]. A spin-wave analysis on a system of N spins, at low temperature gives for the magnetization M [15]

$$M(N,T) = \left\langle \left| \frac{1}{N} \sum_{i=1,N} S_i \right| \right\rangle = \left(\frac{1}{2N}\right)^{1/8\pi K} \tag{1}$$

where $K = J/k_BT$ is the spin-wave stiffness and J is the coupling constant. Equation (1) includes the definition of the magnetization in terms of the *XY* spin vectors S_i.

At this point it is worthwhile clarifying what is meant by finite size. In the original theory of Kosterlitz and Thouless [10] K takes the value $2/\pi$ at T_{KT} and so an order of magnitude estimate for M at T_{KT} is

$$M = (1/2N)^{1/16}.$$

Putting $N = 10^5$ gives $M \simeq 0.47$, indicating that finite-size effects will always be present in the biggest simulations, while putting $N \simeq 10^{16}$–10^{17}, which would correspond to a sample with an area equal to that of this page, still gives $M \simeq 0.1$. It is clear that the thermodynamic limit is inaccessible for the 2D *XY* model, that at low temperatures a magnetization will always be present, and that the variation of M with T should be described by two-dimensional fluctuations.

In layered magnets, only fluctuations on length scales less than the order of $L_{eff} = (J/J')^{1/2}$ are two-dimensional [14, 16], which means that 2D behaviour should occur when the correlation length is less than L_{eff}. Hence much can be learned about the experimental systems, outside the three-dimensional critical region, by studying finite 2D systems of size L_{eff}. Typically J/J' is in the range 10^3–10^4, giving effective finite sizes that can easily be simulated using a work station. In figure 1 we show Monte Carlo simulation results for the magnetization versus temperature of 2D *XY* samples of $N = 1024$ and $N = 10^4$ spins, on a square lattice with periodic boundary conditions. The data were averaged over 3–5 runs with 10^5 Monte Carlo steps per particle per temperature, the first 20,000 of which were used for equilibration. At T_{KT}, RG calculations [17] predict a discontinuous change to a disordered phase with a 'universal jump' to zero in the effective spin-wave stiffness K_{eff} [18]. A magnetization exists in a finite system as long as K_{eff} is non-zero. However, the universal jump is rounded out as the exclusion of length scales greater than L ($= \sqrt{N}$), the system size, means that the spin-wave stiffness is no longer renormalized to zero above T_{KT}. The magnetization falls steeply, yet continuously, and T_{KT} is no longer a special temperature.

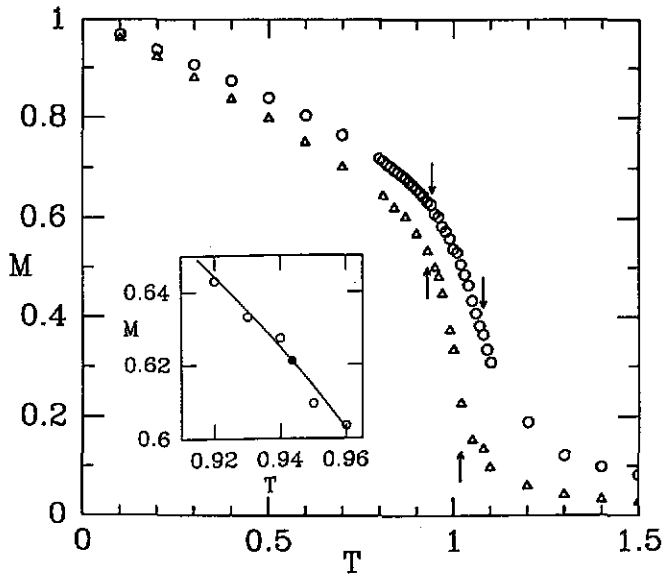

Figure 1. Magnetization versus temperature for a system of $N = 1024$ (open circles) and $N = 10^4$ spins (open triangles). The arrows mark T^* and T_C for each curve, with $T_C > T^*$ (up arrows are for $N = 10^4$; down arrows for $N = 1024$). Inset: behaviour near T^* for $N = 1024$ spins. The line is the theoretical magnetization curve and the full circle is T^* (see text).

To calculate an effective critical exponent β, we need to have a good estimate for M in the region of temperature $\gtrsim T_{KT}$, and to define an effective transition temperature T_C. For this we use the linearized RG equations [11, 17], which we rewrite in a form suitable for finite-size scaling [19]. We then substitute K for the renormalized K_{eff} in the magnetization expression (1). Defining x

$$x = \pi K_{eff} - 2 \tag{2}$$

the RG equations can be solved for $T > T_{KT}$ and small x, to give

$$b_f = \exp\left[\frac{1}{\sqrt{c(T - T_{KT})}}\left(\tan^{-1}\frac{\sqrt{c(T - T_{KT})}}{x_f} - \tan^{-1}\frac{\sqrt{c(T - T_{KT})}}{x_i}\right)\right] \tag{3}$$

where the temperature is in units of J/k_B, b_f is the lattice rescaling parameter, c is a constant ($\simeq 2.1$ [11]), and x_i and x_f are the initial and final values of the parameter x. The direction of the flow is such that $x_i > x_f$. As b_f diverges the initial details are lost and one has [16]

$$x \simeq \frac{\sqrt{c(T - T_{KT})}}{\tan\left[\ln(b)\sqrt{c(T - T_{KT})}\right]}. \tag{4}$$

By making the substitution $L \simeq b$, we can calculate the properties of a finite system of size L, and then use L as the rescaling parameter [19]. In the finite system the point at which $x = 0$, giving $K_{\rm eff}$ its universal value $2/\pi$ [11], occurs at a shifted temperature T^*

$$T^*(L) \simeq T_{\rm KT} + \frac{\pi^2}{4c(\ln L)^2}. \tag{5}$$

Unlike in the case of the infinite system, $\mathrm{d}K_{\rm eff}/\mathrm{d}T$ is finite at the temperature T^*, so one choice of $T_{\rm C}$ is the temperature at which $K_{\rm eff} = 0(x = -2)$. A more realistic choice is the temperature at which the correlation length, ξ, becomes equal to the system size. For the infinite system and for $T > T_{\rm KT}$, Kosterlitz [11] defined ξ as the value of the rescaling parameter at which there is a significant deviation from fixed-point behaviour, that is, x no longer close to zero. The deviation from $x \simeq 0$ is sudden, and ξ is identified by putting the argument of the tangent in (4) equal to π, giving

$$\xi \simeq \exp\left(\frac{\pi}{\sqrt{c(T - T_{\rm KT})}}\right). \tag{6}$$

The quantitative validity of (6) is confirmed by the results of Gupta *et al* [20]. With $L \simeq \xi$ one finds

$$T_{\rm C}(L) \simeq T_{\rm KT} + \frac{\pi^2}{c(\ln L)^2}. \tag{7}$$

For large L, the difference between these two choices of $T_{\rm C}$ becomes negligible compared with the shift $T_{\rm C} - T^*$.

Expression (1) for M is derived by summing spin-wave contributions over all wavelengths up to L and so is exact if the spin-wave stiffness is independent of wavelength, which is not the case in the presence of vortices. However, the summation is dominated by the long-wavelength components, and so we may replace K in (1) by $K_{\rm eff}$ if the spin-wave stiffness varies sufficiently slowly with wavelength. This condition is met in the finite system for $T \gtrsim T^*$.

We define the exponent β as

$$\beta(L,T) = \left[\frac{\partial \ln M(L,T)}{\partial \ln(t(L))}\right]_L \tag{8}$$

where $t = T_{\rm C} - T$. As L becomes very large, there is no error incurred by replacing K by $K_{\rm eff}$ in (1), and making (4)–(7) into equalities. At $t^* = T_{\rm C} - T^*$, we arrive, after some algebra, at a quite remarkable universal result:

$$\beta(L,T^*) = \frac{3\pi^2}{128} = 0.231\ldots. \tag{9}$$

As $L \to \infty, T_{\rm C}$ and T^* converge on $T_{\rm KT}$, the magnetization disappears, and the behaviour passes smoothly to that of KT theory. However the result (9) remains valid until the limit, at which point β becomes undefined. The calculation gives the universal value at T^* only, and we anticipate that the range of temperature over

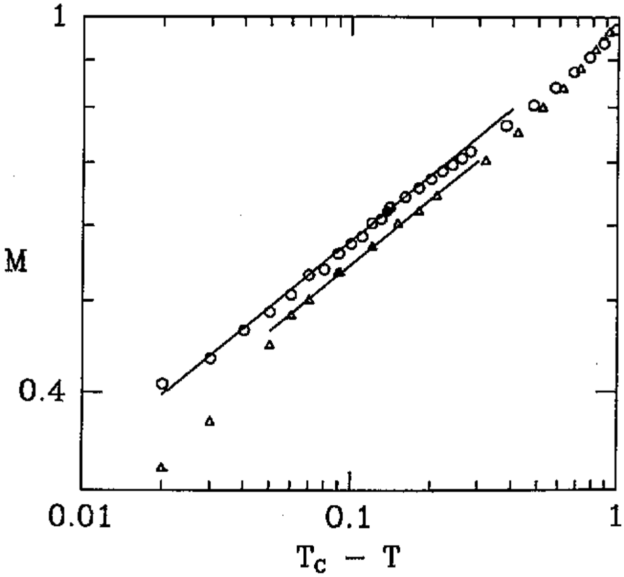

Figure 2. $\log_{10} M$ versus $\log_{10}(T_C - T)$ for $N = 1024$ (open circles) and $N = 10^4$ (open triangles) spin systems. Full points: theoretical T^*, and the lines are of slope $\beta = 3\pi^2/128$.

which (9) is a good estimate for β will be non-universal. For finite L, the various approximations in the calculation introduce corrections to β of order $\beta/\ln(L^2)$. These are not negligible for the system sizes studied $(0.23/\ln(1024) \simeq 0.02)$, and it is clear that one can only have full confidence in this result for very large system sizes, where corrections are negligible term by term. However, the individual terms cancel out to some extent, and the validity of the calculation for these relatively small systems can be tested directly by comparison with Monte Carlo data.

The above results give us a recipe for choosing T_C for the numerical results. First we calculate the temperature at which $M = (1/2N)^{1/16}$, corresponding to $x = 0$ and $K_{\text{eff}} = 2/\pi$. This locates T^*, and defines T_C following

$$T_C - T_{KT} = 4(T^* - T_{KT}) \tag{10}$$

the best estimate for T_{KT} being 0.898 [20]. We can test the consistency of this argument by calculating the constant c from equation (5). Kosterlitz [11] gives $c \simeq 2.1$, and from the parameter b_ξ of Gupta *et al* [20,21], $c \simeq 2.35$ in the paramagnetic region.

Using this recipe on the data for the 1024-spin system gives $T^* = 0.943 \pm 0.001$ (see inset, figure 1), $T_C = 1.080 \pm 0.004, c = 2.48$. A pragmatic choice of T_C to give the best power-law behaviour gives $T_C = 1.080 \pm 0.002$, in very accurate agreement. An analysis on the 10^4-spin system is also in accurate agreement with the calculation, with $c \simeq 2.2$. For both systems T_C is confirmed to be close to the point where the magnetization starts to develop (see figure 1). Plots of $\log M$ versus $\log(T_C - T)$ are shown in figure 2, where the straight lines have slopes of $3\pi^2/128$. To within the uncertainty on c, the lines of figure 2 and figure 1 (inset) describe the data at T^* with no adjustable parameters. A comparison of the data for the two systems in figure 2 shows how non-universal spin-wave behaviour gives way to universal scaling behaviour near T^*. The range of $\beta \simeq 0.23$ is smaller for the bigger system.

In addition to the interplanar coupling J', real materials often have a weak n-fold crystal field h_n, but to our knowledge, only the case of h_4 has been studied in detail [22]. It appears that $L_{\rm eff}$ is determined by J' even when $h_4 \gg J'$, which is consistent with h_4 being a marginal variable [17]. For a general weakly perturbed system, the spontaneous magnetization vanishes with a critical behaviour characteristic of the perturbation. At low temperatures, once the correlation length drops below the length scale required to make the perturbation relevant, all that is left are 2D fluctuations.

The results of figure 2 are consistent with the range of $\beta \simeq 0.23$ in layered magnets, where $J/J' \simeq 10^3$–10^4 (see table 1). These estimates of β were measured relative to the 3D ordering temperature T_{3D}. $\beta = 0.23$ is observable because the small extent of the 3D critical region ensures that $T_C \simeq T_{3D}$, and that T^* is outside the 2D–3D crossover region. The temperature at which $\eta = \frac{1}{4}$ [11], which we now interpret as T^*, has been located in experiments on K_2CuF_4 [5], Rb_2CrCl_4 [8] and $Rb_2CrCl_2Br_2$ [22], and in previous computer simulations [24]. In future publications we shall present a detailed analysis where we demonstrate agreement between experiment and theory for all these systems [7,23].

Our principal conclusion is that $\beta = 0.23$ is a property of the 2D *XY* model that is observed in real systems. The general predictions of our calculation agree with experiment and computer simulations to a high degree of accuracy, although this is perhaps surprising, given the expected logarithmic errors. Our results strongly suggest that KT theory is relevant to real magnets.

It is a pleasure to thank J-L Barrat, M J P Gingras and R B Stinchcombe for useful discussions.

References

[1] Kosterlitz J M and Thouless D J 1978 *Prog. Low Temp. Phys.* **VIIIB** 373
Nelson D R 1983 *Phase Transitions* vol 7, ed C Domb and K L Lebowitz (New York: Academic) p 1
Minnhagen P 1987 *Rev. Mod. Phys.* **59** 1001

[2] Regnault L P and Rossat-Mignod J 1990 *Magnetic Properties of Layered Transition Metal Compounds* ed L J de Jongh (Deventer: Kluwer) pp 271, 281.

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

[4] Hirakawa K and Ikeda H 1973 *J. Phys. Soc. Japan* **35** 1328

[5] Hirakawa K and Ubukoshi K 1981 *J. Phys. Soc. Japan* **50** 1909

[6] Hutchings M T *et al* 1981 *J. Phys. C: Solid State Phys.* **14** 5327

[7] Als-Nielsen J, Bramwell S T, Hutchings M T, McIntyre G J and Visser D 1992 Preprint ILL

[8] Cornelius C A *et al* 1986 *J. Phys. C: Solid State Phys.* **19** 909

[9] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133

[10] Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Berezinskii V L 1971 *Sov. Phys.–JETP* **32** 493

[11] Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046

[12] Kawabata C and Bishop A R 1986 *Solid State Commun.* **60** 167
Volkel A R *et al* 1991 *Phys. Rev.* B **44** 10066

[13] The transition metal formates are often regarded as 2D Heisenberg magnets, but the evidence presented in this paper suggests that they should be regarded as *XY*-like. We shall discuss experimental evidence of this in a future publication.

[14] Berezinskii V L and Blank A Ya 1973 *Sov. Phys.–JETP* **37** 369

[15] Tobochnik J and Chester G V 1979 *Phys. Rev.* B **20** 3761

[16] Hikami S and Tsuneto T 1980 *Prog. Theor. Phys.* **63** 387
These authors obtain equations similar to (4), (6), (7) for the analogous case of interplanar coupling (see also [1]).
[17] José J V *et al* 1977 *Phys. Rev.* B **16** 1217
[18] Nelson D R and Kosterlitz J M 1977 *Phys. Rev. Lett.* **39** 1201
[19] Binder K 1986 *Monte Carlo Methods (Springer Topics in Current Physics 7)* (Berlin: Springer) p 370
[20] Gupta R *et al* 1988 *Phys. Rev. Lett.* **61** 1996
[21] In estimating c from numerical data we adjust for the difference between the Monte Carlo result $T_{KT} = 0.898$ [20], and the RG result $T_{KT} = 1.35$ [11, 17]. The c we quote is that derived from the data through equation (6) multiplied by 0.898/1.35.
[22] Bramwell S T 1989 *DPhil Thesis* Oxford University
[23] Bramwell S T and Holdsworth P C W unpublished
[24] Carpenter D B and Chalker J T 1989 *J. Phys.: Condens. Matter* **1** 4097
[25] Chattopadhyay T *et al* 1992 *J. Magn. Magn. Mater.* **104–107** 607
[26] Bramwell S T *et al* 1986 *Inorg. Chem.* **25** 417
[27] Koyama K, Nobumasa H amd Matsuura M 1987 *J. Phys. Soc. Japan* **56** 1553