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Magnetic fluctuations in a finite two-dimensional XY model

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Abstract. We calculate the two-dimensional probability $P(M_x, M_y)$ for the magnetization in a two-dimensional XY model of finite size. We show that, for arbitrarily large N, there is a topological difference between the distributions in the low-temperature spin wave regime and in the high-temperature paramagnetic regime. In the low-temperature phase $P(M_x, M_y)$ is a well-defined ring function and we calculate an upper bound for $P(0,0) \leqslant 0.0019(T/J)^2$. Even so, this is consistent with the susceptibility per spin, χ, being divergent. We show further that the distribution function $Q(M)$ for the scalar magnetization has a universal form, scaling with the single variable $y = JT^{-1}ML^{T/4\pi J}$, where L is the system size and J is the coupling constant. We show that χ has considerable structure, with two terms of order N, one due to the spin waves and the other due to vortices. This leads to a peak in χ at the Kosterlitz–Thouless–Berezinskii transition.

1. Introduction

The finite-size two-dimensional (2D) XY model is an appealing system for theoretical study as it shows critical behaviour over a range of temperatures below the Kosterlitz–Thouless transition temperature T_{KT}, is extremely accessible to analytic techniques and is of broad experimental relevance [1, 2]. The model is defined with the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \tag{1}$$

where J is the ferromagnetic coupling constant and θ_i is the angle of orientation of spin vector $\boldsymbol{S}_i$, constrained to lie in a plane. The summation is over nearest neighbours and we take the spins to be on the sites of a square lattice with periodic boundary conditions. We use a system of units with Boltzmann's constant k_B equal to unity throughout.

The critical nature of the low-temperature phase gives the 2D XY model the intriguing property that in a realizable macroscopic system not all the physically observable quantities can be described by taking the thermodynamic limit. In particular, true long-range magnetic order is excluded for any temperature by the Mermin–Wagner theorem [3]. However, at low temperature the finite-size L provides a cut off for the divergent correlation length, giving

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a substantial finite-size magnetization per spin $M(L)$ [4, 5]. The latter is not a true order parameter, as it is not an intensive quantity; however, it goes to zero so slowly with system size that it only approaches zero on a planetary length scale. Thus, the thermodynamic limit is inaccessible with respect to the pair of conjugate thermodynamic variables, magnetization $\boldsymbol{M}$ and field $\boldsymbol{H}$, even though it is perfectly accessible with respect to internal energy U, entropy S and temperature T. Finite size is not the only way to introduce a cut off at small wave vector and so restore the magnetization. Weak coupling to the third dimension, spin anisotropy or weak crystal fields can have equivalent effects [4, 6].

Such effects are common in 2D systems, and were first pointed out in the 1930s by Peierls [7]. They have also been discussed by, for example, Landau and Lifshitz [8], Mermin [9], Berezinskii and Blank [10] and several other authors [11]. We have illustrated that the magnetic order observed in real 2D XY systems is a direct result of finite-size corrections [5]. Such experimental systems show a remarkable universal property, that is a power law dependence of the magnetization on temperature, with exponent $\beta \approx 0.23$ [1]. Using the renormalization equation of Kosterlitz for the spin wave coupling $K = J/T$, we calculated the finite-size magnetization in the region of the Kosterlitz–Thouless–Berezinskii transition, and identified a finite-size critical region bounded between temperatures $T^*(L)$ and $T_{\mathrm{C}}(L)$. T^* is the shifted T_{KT} in the sense that at this temperature the vortex distribution renormalizes in a self-similar manner on length scales up to L, the system size. $T_{\mathrm{C}}(L)$ is the temperature at which the correlation length equals L, and corresponds to the standard definition of a critical temperature for a finite system [12]. We found power law behaviour for the magnetization as a function of $t = T_{\mathrm{C}}(L) - T$, with universal exponent $\beta = 3\pi^2/128 = 0.2312\ldots$, in agreement with numerous experiments [1]. The temperatures $T_{\mathrm{C}}(L)$ and $T^*(L)$ can both be measured experimentally, and the values confirm our theoretical predictions extremely well [14, 16].

As this finite-size magnetization is of direct physical relevance, and is so surprisingly reminiscent of a true order parameter, it is of interest to investigate its properties further. In section 2 we calculate the probability distribution for the finite-size magnetization, and its first and second moments. We can expect that this distribution is non-Gaussian in the low-temperature regime, as this is a specific property of a critical system. We find, in fact, the distribution function $P(M_x, M_y)$, where M_x and M_y are the two components of the order parameter, does not approach a 2D Gaussian function centred on $M_x = M_y = 0$, even in the thermodyamic limit. Rather it remains a well-defined ring function, with probability maximum at a value $M(L) = \sqrt{M_x^2 + M_y^2}$ and a minimum at the origin. We discuss, further, the universal properties of this function. This has consequences for the susceptibility which, as is well known, is divergent at all temperatures below T_{KT}. One of our main results is that susceptibility, although divergent in the sense that it scales with the system size, remains numerically quite small, and should be measurable in a practical system†. This 'infinite' susceptibility furthermore has a non-trivial temperature dependence, again reminiscent of a second-order phase transition. In section 3 we explore the physical origin of this temperature dependence, and conclusions are drawn in section 4.

† We have previously argued that the system size relevant to magnetic experiments rarely exceeds 10^6 spins, as they are limited by symmetry-breaking perturbations. It is possible that liquid Helium film experiments could provide larger system sizes, see [15].

2. Fluctuations in the low-temperature regime

The physics of the 2D XY model is dominated by two types of excitation: harmonic spin waves and spin vortices [4, 17–20]. The latter map onto a neutral 2D Coulomb gas in the grand canonical ensemble, with the temperature scale of the fugacity set by the coupling constant J. At $T_{\rm KT}$ pairs of vortices of opposite 'charge' unbind and the high-temperature phase constitutes a gas of free charges.

It is desirable to study models which support only those excitations pertinent to the problem, namely harmonic spin waves and vortex pairs, while maintaining the full XY symmetry. A generic model of this type is the Villain model [21], which is the basis of systematic renormalization group calculations [17, 19, 20]. In this paper we study what we refer to as the harmonic XY, or HXY, model [14]. Its Hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} [1 - \tfrac{1}{2}(\theta_i - \theta_j - 2\pi n)^2] \tag{2}$$

where $n = 0, \pm 1$ is an integer chosen so that $(\theta_i - \theta_j - 2\pi n)$ lies between $\pm\pi$. This model is almost equivalent to the Villain model [21], but is more practical from a numerical point of view, as the vortex variable n is not a thermodynamic variable, but is constrained to the values $n = 0, \pm 1$ [19]. It is found that the neglect of the anharmonic but analytic terms in the development of the cosine interaction results in accurate agreement between numerical and renormalization group estimates for $T_{\rm KT}$ [22]. In fact the theoretical prediction of $T_{\rm KT} = 1.350\,85J$ appears to be exact. At temperatures which are small compared with $T_{\rm KT}$ the vortex density is exponentially small and the HXY model reduces to the harmonic spin wave, or Gaussian model, which is solved exactly in the appendix.

It is convenient to define an instantaneous scalar order parameter M

$$M = \frac{1}{N}\sqrt{\left(\sum_{i=1,N} \boldsymbol{S}_i\right)\left(\sum_{i=1,N} \boldsymbol{S}_i\right)}. \tag{3}$$

The Mermin–Wagner theorem applies to the thermal average $\langle M \rangle$ [3, 2]. In the appendix we derive, using spin wave theory, the following result for the magnetization $\langle M \rangle$, exact to leading order in N:

$$\langle M \rangle = \left(\frac{1}{2N}\right)^{T/8\pi J}. \tag{4}$$

We also show that the susceptibility per spin, defined as

$$\chi = \frac{N}{T}(\langle M^2 \rangle - \langle M \rangle^2) \tag{5}$$

is given by the expression

$$\chi = \frac{\langle M \rangle^2}{T} \sum_r \left[\exp\left(\frac{T}{J} \times G(r)\right) - 1\right] \tag{6}$$

where $G(r)$ is the lattice Green's function for a square lattice (see the appendix). To an excellent approximation one finds

$$\chi = \frac{1}{2a_{\rm 2D}} \frac{N\langle M \rangle^2 T}{J^2} \qquad a_{\rm 2D} = 258.6 \tag{7}$$

with the susceptibility per spin therefore diverging as $\chi \sim N^{1-T/4\pi J}$.

In figure 1 we show the initial evolution, in Monte Carlo time, of the vector magnetization in the x–y plane, for a 1024 spin system at $T/J = 1$, starting from a

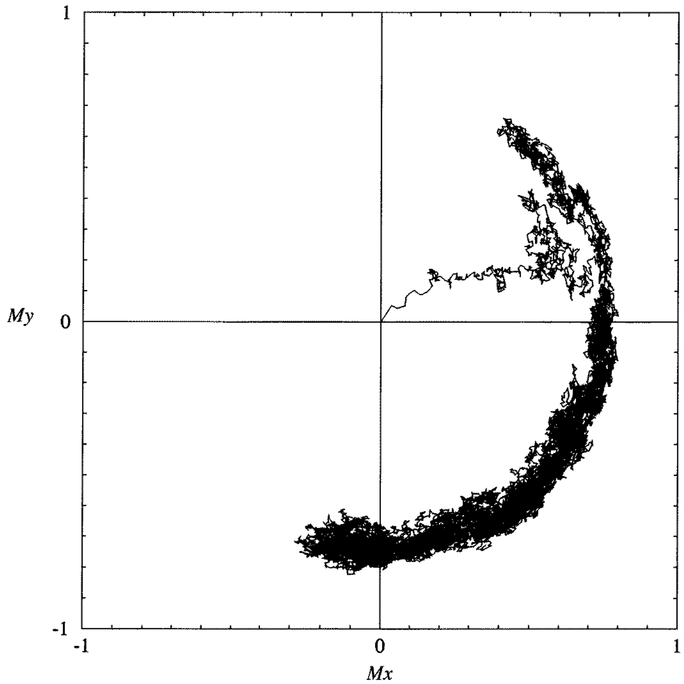

Figure 1. Initial evolution, in Monte Carlo time, of the vector magnetization $M = (M_x, M_y)$ in the x–y plane, for a 1024 spin system at $T/J = 1$, starting from a random configuration with $M = 0$. The random walk is shown for the first 20 000 Monte Carlo time steps per particle which illustrates the timescale on which the magnetization revolves.

random configuration. This is still in the low-temperature phase, where the vortex density is negligibly small and the system is perfectly described by harmonic spin waves. One can see that the system escapes rapidly from the origin. After the transient effects have died away the order parameter fluctuates about a well-defined mean and never returns close to the origin, while the direction of magnetization changes in a relatively short time. The walk is shown for the first 20 000 Monte Carlo time steps (MCS) per particle which illustrates the timescale on which the magnetization revolves. It should be noted that the simulations used to calculate thermal properties, described below, used about 10^7 MCS, the first 10^5 steps being used only for equilibration.

From figure 1, the scalar magnetization therefore appears to be a well-defined quantity despite its fluctuations, as measured by the susceptibility, being divergent in the thermodynamic limit. From equation (7) we see that it is well-defined because the prefactor of the 'divergent' susceptibility is small and goes to zero as T goes to zero. The normalized standard deviation of the distribution,

$$\frac{\sigma}{\langle M\rangle} = \sqrt{\frac{\langle M^2\rangle - \langle M\rangle^2}{\langle M\rangle^2}} = \frac{\sqrt{N\chi T}}{N\langle M\rangle} \tag{8}$$

has a numerical value of only $\approx 0.04T/J$, but is independent of system size. In a non-critical system, with finite correlation length one expects $\sigma/\langle M\rangle$ to go to zero as $N^{-1/2}$ in the large N limit. We remark that even in three dimensions this criterion is not quite satisfied for the XY model and we find that $\sigma/\langle M\rangle$ varies as $N^{-1/3}$ only (see the appendix).

We can parametrize the vector magnetization in terms of Cartesian components M_x, M_y

or in terms of M and the angle in the plane ϕ, from which we define the probability distributions $P(M_x, M_y)$ and $Q(M, \phi)$. From the symmetry of the Hamiltonian $Q(M, \phi)$ is separable, with $Q(M, \phi) = 1/2\pi Q(M)$. This is clearly illustrated in figure 1. The distributions P, and Q are therefore related

$$P(M_x, M_y) = \frac{1}{2\pi M} Q(M) \qquad M^2 = M_x^2 + M_y^2 \tag{9}$$

and σ gives the width of the distribution $Q(M)$.

If the system exhibited a standard second-order phase transition we would expect $P(M_x, M_y)$ to change form as one passes through T_C [12]. At high temperatures it should be a function centred at the origin, and with width varying as $1/N^{1/2}$. Such a narrow distribution is represented to an excellent approximation by a Gaussian function. At low temperatures the distribution should change to a ring function whose radial cross section $P(M, 0)$ should be a bimodal distribution with sharp peaks centred at $M_x = \pm\langle M\rangle$. A Gaussian function comes from the first term in a Landau expansion for the free energy $F(M)$. At the critical point the Landau expansion is invalid, and the susceptibility is divergent, from which we expect to find that $P(M, 0)$ is non-Gaussian, with a width of order unity.

We have calculated $Q(M)$ from Monte Carlo simulation, from which we can reconstruct $P(M, 0)$, for the 2D HXY model of size $N = 1024$ and $N = 10\,000$ and for a three-dimensional (3D) HXY system of size $N = 1000$ spins. The number of MCS was typically 10^7 per temperature. Relaxation times of 10^5 MCS were found to be sufficient to reach equilibrium at all temperatures.

In figure 2 we show $P(M, 0)$ for $T/J = 0.5, 1.0$, $T^*/J = 1.46$ and $T_C/J = 1.79$

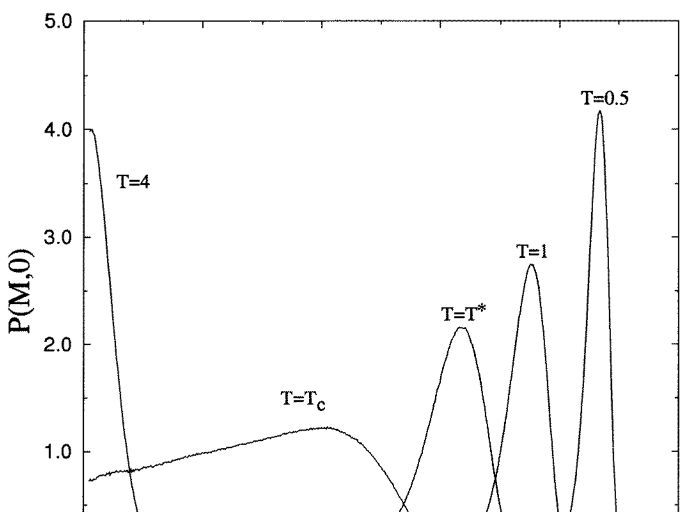

Figure 2. Probability distribution for the magnetization of the finite 2D HXY model, $P(M, 0)$, for $T/J = 0.5, 1.0$, $T^*/J = 1.46$ and $T_C/J = 1.79$ for $N = 1024$ spins. The area under the curves is not normalized, as it represents a slice through a 2D distribution. The volume swept out by the curve when rotated in the plane through 2π is correctly normalized. These data should be compared with equivalent curves for three dimensions, shown in figure 3.

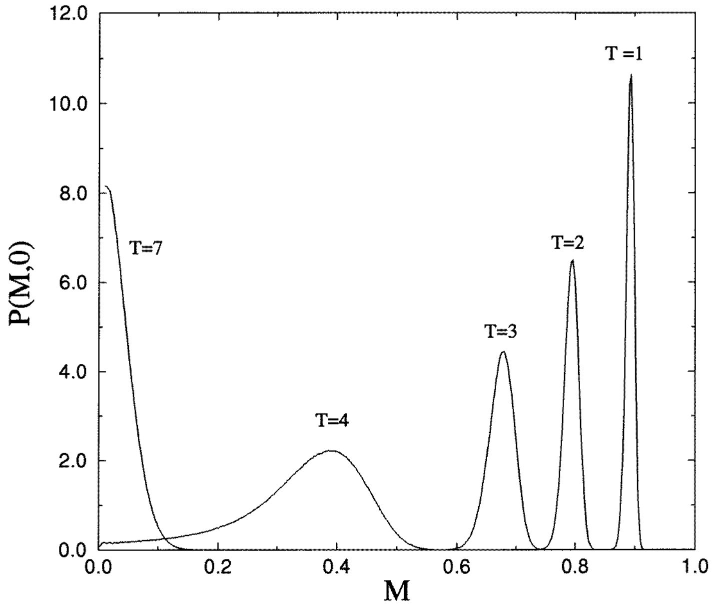

Figure 3. Probability distribution for the magnetization of the finite 3D HXY model, $P(M, 0)$, for $T/J = 1, 2, 3, 4, 7$, for $N = 1024$ spins. The area under the curves is not normalized, as it represents a slice through a 2D distribution. The volume swept out by the curve when rotated in the plane through 2π is correctly normalized.

for $N = 1024$ spins. These data should be compared with equivalent curves for three dimensions, shown in figure 3. The 3D system follows exactly the scenario outlined above. For the 2D system the distribution at T_C has a finite value at the origin, $M_x = 0$, $M_y = 0$, just as for three dimensions. At lower temperatures the probability of finding the magnetization at the origin goes to zero, as already observed in figure 1. However, despite the well-defined finite-size magnetization, the distribution remains wider than in three dimensions and is asymmetric, with a tail in the distribution for $M < \langle M\rangle$. This is consistent the 2D system remaining critical throughout the low-temperature spin wave regime. The system can have both a divergent susceptibility and a well-defined finite-size magnetization because of the very small prefactor in equation (7).

In figure 4 we compare $P(M, 0)$, for the 2D and 3D distributions, with a Gaussian fit using the first two moments, as calculated in equations (4) and (6). In two dimensions the discrepancies are large, particularly in the tails of the distribution. For $M > \langle M\rangle$ the distribution is steeper than the fit, while for $M < \langle M\rangle$ there is a long tail extending to smaller values of M than those offered by the Gaussian. The tail in the distribution, at the temperature shown, of $T/J = 1.0$, is entirely due to spin wave excitations and not to vortices. The vortex density at this temperature is exponentially small and does not make a significant contribution to the distribution. That the spin waves alone can produce the tail is consistent with the system being critical throughout the spin wave regime, with fluctuations towards configurations with $M < \langle M\rangle$ having a limitingly small cost in free energy. As the temperature is increased and vortices do appear they give access to configurations at smaller magnetization and the tail is extended towards the origin [23]. This can be seen by comparing curves for $T/J = 1$ and $T/J = 1.46$ in figure 2. In three dimensions the Gaussian fit is much improved, particularly in the wings of the distribution and the behaviour

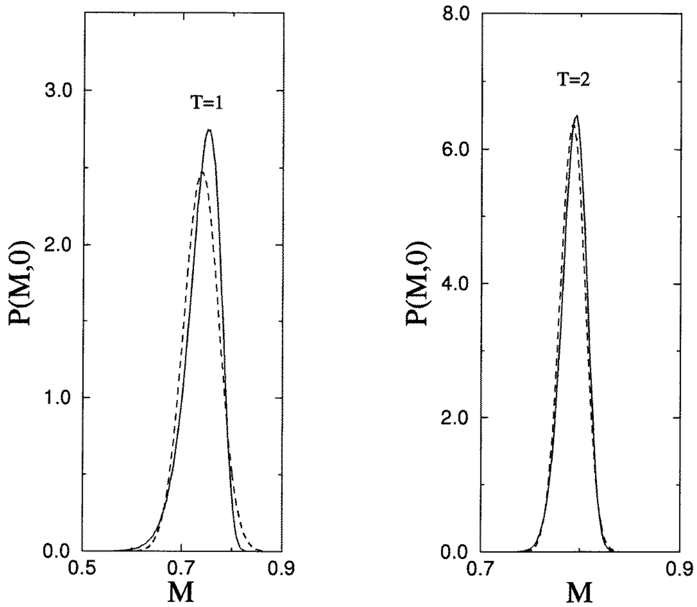

Figure 4. Probability distribution (full curve) for the magnetization of the finite 2D HXY model, $P(M, 0)$, for $T/J = 1$, (*a*) and of the finite 3D HXY model, $P(M, 0)$, for $T/J = 1$, (*b*) for $N = 1024$ spins. The broken curve represents a Gaussian fit using the first two moments of the distribution, calculated from spin wave theory.

conforms closely to predictions for an ordered, non-critical system.

The exact result (4) confirms scaling arguments for the magnetization at a critical point [12], $\langle M \rangle \sim L^{-\beta/\nu}$, with β and ν the relevant critical exponents. Despite the fact that a conventional β and ν do not exist for the 2D XY model, their ratio $x = T/4\pi J$ is perfectly well defined through equation (4) for all temperatures $T \leqslant T^*$. At T^* the scaling relation

$$x = \beta/\nu = \frac{d}{\delta + 1} = \frac{1}{8} \tag{10}$$

is satisfied by putting $T/J \approx \pi/2$, which is the mean-field approximation for T_{KT} [18]. More precisely, we have shown [5] that the renormalization of the temperature due to vortices is taken into account correctly, by replacing T/J with the effective temperature $(T/J)_{\mathrm{eff}} = \pi/2$ at T^*, in which case the scaling relation is satisfied exactly.

The distribution function for the magnetization at a critical point has been discussed by several authors [12, 13]. Binder [12] argued, using the example of an Ising system with distribution $P_L(M)$, that within the critical region

$$P_L(M) = L^{\beta/\nu} P(L/\xi, ML^{\beta/\nu}) \tag{11}$$

where ξ is the correlation length. ξ is the length scale at which one can expect a cross over to a non-critical regime with Gaussian fluctuations. Very close to the critical point the correlation length of the infinite system would be much bigger than the system size L. In this situation one expects self-similar behaviour, with L being the only important scale above the microscopic length. P_L should therefore depend on the single variable $ML^{\beta/\nu}$.

In our case we have a line of critical points for all temperatures less than T_{KT} with temperature-dependent exponents. If the universal function is to be the same at different critical points one should expect an explicit temperature dependence despite there being no

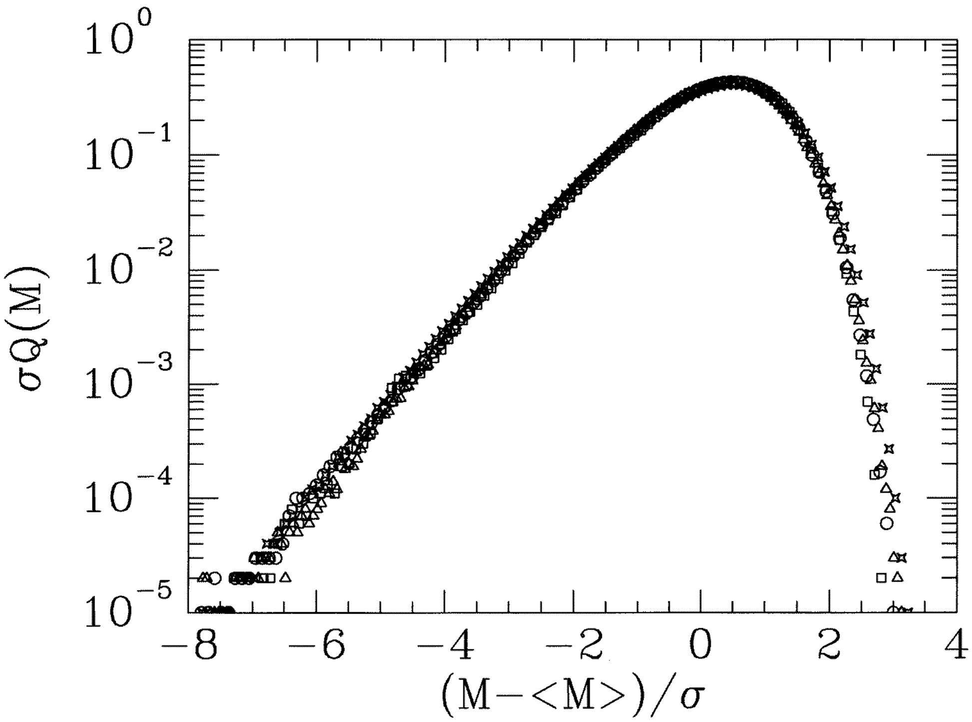

Figure 5. $\log(\sigma Q(M))$ versus $(M - \langle M\rangle)/\sigma$ for $T/J = 0.5$ for $N = 100$ (stars), $N = 1024$ (circles), $N = 10\,000$ (squares), and for $T/J = 1.0$ for $N = 1024$ (triangles).

correlation length. In figure 5 we plot $\log(\sigma Q(M))$ versus $(M - \langle M\rangle)/\sigma$ for $N = 10^2$, 10^3 and 10^4 spins at $T/J = 0.5$ as well as for $N = 10^3$ spins at $T/J = 1.0$. The data clearly fall on a universal curve over five orders of magnitude. We define a reduced variable $y = M/\sigma \sim JT^{-1}ML^{T/4\pi}$, with $\overline{y} = \langle M\rangle/\sigma \sim JT^{-1}$ which is independent of L. Our universal function is therefore of the form $Q(y - \overline{y})$. We observe corrections to universality for systems containing less that 100 spins.

As one approaches T^*, and vortex pairs become excited in appreciable numbers, the asymmetric tail to the distribution becomes more pronounced and the data no longer fall on the universal curve. In this regime there are two independent contributions to the critical fluctuations, as is discussed further in the next section.

As the magnetization is zero in the thermodynamic limit it is of interest to calculate the probability, $P(0,0)$, of finding M 'tunnelling' to the origin. As the standard deviation $\sigma \ll \langle M\rangle$ in the spin wave regime, we can write, to an excellent approximation

$$P(M,0) \approx \frac{1}{2\pi\langle M\rangle} Q(M) \tag{12}$$

which means that σ^2 is the variance of both distributions. Within this approximation we can now calculate an upper bound on the probability $P(0,0)$ using Chebyshev's inequality

$$P(0,0) \leqslant \frac{\sigma^2}{\langle M\rangle^2} = 0.0019\left(\frac{T}{J}\right)^2 \tag{13}$$

which is independent of system size.

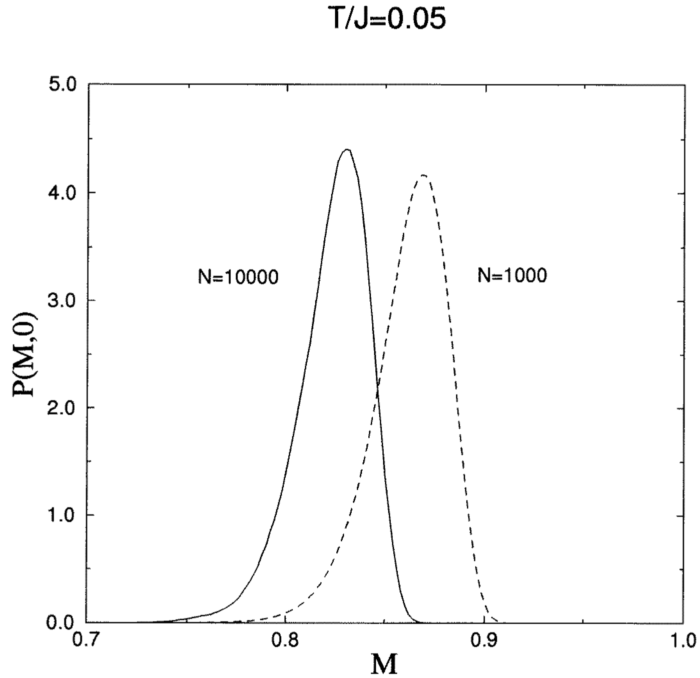

Figure 6. The probability distribution for the magnetization of the finite 2D HXY model, $Q(M)$, as a function of system size N for $T/J = 0.5$. The curves shown correspond to $N = 1024$ and $N = 10\,000$ spins.

The actual value may well be much less than this bound as is clearly indicated from figures 1 and 2. However, equation (13) shows that even in the thermodynamic limit the probability of the magnetization tunnelling to the origin is extremely small for all temperatures $T < J$. As N increases the mean magnetization shifts towards the origin, but at the same time the width of the distribution falls to zero. As a result the distribution remains a well-defined ring function right to the thermodynamic limit and one never, for any system size, has a distribution function centred on the origin, as in the paramagnetic regime. This result gives a clear practical meaning to the topological long-range order [18] in the 2D XY model; the finite-size magnetization is precisely defined for arbitrarily large system size, even though the amplitude goes to zero.

The effect of the distribution narrowing with increasing system size is illustrated in figure 6, where we show $P(M, 0)$ for $N = 1024$ and $N = 10\,000$ at $T/J = 0.05$.

3. Fluctuations near the Kosterlitz–Thouless–Berezinskii phase transition

In this section we consider in more detail the behaviour of the susceptibility χ as one leaves the spin wave regime and passes through the Kosterlitz–Thouless–Berezinskii transition. In figure 7 we show Monte Carlo data for χ for 1024 spins, as a function of temperature. The low-temperature result, equation (7), is seen to fit the data very accurately up until $T \approx J$. Above this temperature vortex pairs are excited in appreciable numbers, and one observes a sharp rise, with a maximum at a temperature $T_C(L)$ [5]. This corresponds to the temperature in figure 2 at which the probability distribution broadens. In this section we

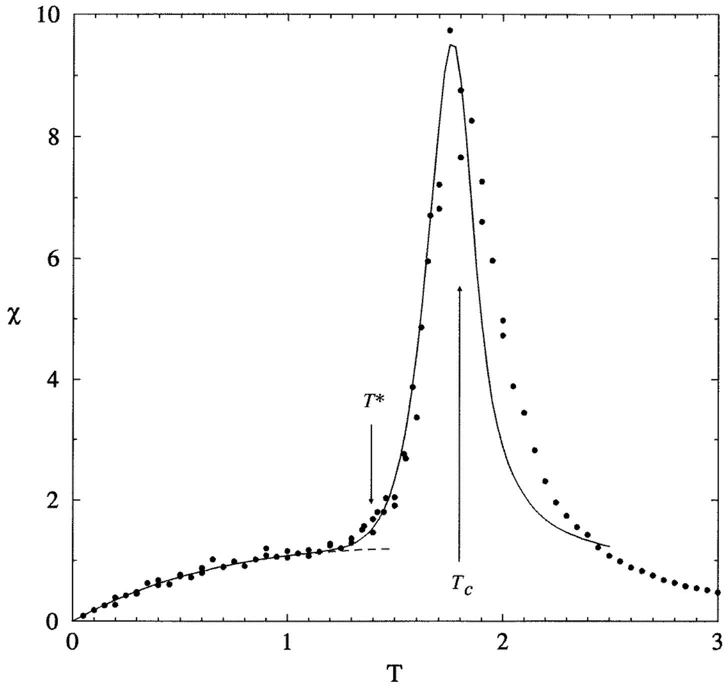

Figure 7. Susceptibility versus temperature for the finite 2D HXY model, with $N = 1024$ spins. Circles represent the Monte Carlo data, the broken curve is expression (7) and the full curve is the result of the real-space renormalization group calculation, as described in the text.

present arguments to identify the physical origin of the susceptibility peak.

The peak in the susceptibility cannot be explained by simply replacing T by a vortex-renormalized T' in equation (15). It is easily verified that this does not give the required divergence, even if $T \to \infty$. Rather, the peak represents a second divergence of order N in addition to that due to the harmonic spin waves. It means that a new length scale is introduced into the problem by the vortices, which one can see by writing the susceptibility

$$\chi T = \sum_r g(r) - \langle M \rangle^2 \tag{14}$$

where $g(r)$ is the two-spin correlation function. To obtain a divergence of order N requires a non-zero contribution from each term in the summation in equation (14). Defining ξ as the length scale at which $g(r > \xi) = \langle M \rangle^2$, then the susceptibility is given by $\chi \sim \xi^2$, and a divergence of order N implies that $\xi \to L$.

In the spin wave regime χT takes the form (see the appendix)

$$\chi T \approx \sum_r \exp\left(-K^{-1}G(0)\right)\left(1 + \tfrac{1}{2}K^{-2}G(r)^2\right) - \langle M \rangle^2 \tag{15}$$

where $K = J/T$. The 'infinite' susceptibility but with small amplitude arises because $\exp\left(-K^{-1}G(0)\right) = \langle M \rangle^2$ leaving one with

$$\chi T \approx \sum_r \frac{1}{2} \exp\left(-K^{-1}G(0)\right) K^{-2} G(r)^2 = \frac{N \langle M \rangle^2 K^{-2}}{2a_{2D}}. \tag{16}$$

The principle effect of the vortex pairs, excited in appreciable numbers above $T \sim J$, is to soften the spin wave modes. The spin stiffness at wavevector q is changed from $q^2 K$ to an effective value $q^2 K_{\text{eff}}(q)$, and with this the full expression for the susceptibility becomes

$$\chi T \approx \sum_r \exp(-K_{\text{eff}}^{-1}(r)G(0))(1 + \tfrac{1}{2}K_{\text{eff}}^{-2}(r)G(r)^2) - \langle M \rangle^2. \tag{17}$$

If K_{eff}^{-1} varies with r then $\exp(-K_{\text{eff}}^{-1}(r)G(0))$ is no longer equal to $\langle M \rangle^2$ and one finds a second contribution to the divergent susceptibility whose amplitude can be much larger than the spin wave term. This second correlation length is therefore directly related to the length scale over which $K_{\text{eff}}(r)$ changes with r, and ξ may be interpreted as the length beyond which $K_{\text{eff}}(r)$ is approximately constant.

We can calculate $K_{\text{eff}}(r)$ to a very good approximation using the renormalization group theory for the 2D XY model [17, 19] and in what follows we use the nonlinear real space renormalization equation of José *et al* [19], which gives us directly an expression for $K_{\text{eff}}^{-1}(r)$

For $T \leqslant J$, $K_{\text{eff}}(r)$ is equal to the unrenormalized spin wave coupling $K = J/T$ for all r. For $J < T < T_{\text{KT}}$ the effect of the renormalization is very small for the system sizes we consider, as can be seen from figure 6 and it is only above T_{KT} that the second term has an appreciable effect. In the thermodynamic limit T_{KT} is the fixed point for vortex renormalization and it marks the dividing line between renormalization of $K_{\text{eff}}(\infty)$ to a new constant value and to zero. This is the universal jump of K_{eff} from $2/\pi$ to zero. Above T_{KT}, $K_{\text{eff}}(r)$ remormalizes in an extremely nonlinear fashion, staying asymptotically close to the universal value of $2/\pi$ before shooting to zero at a length scale L_{C}, which Kosterlitz identified as the correlation length [17] and from which we define $T_{\text{C}}(L)$. We therefore conclude that for a finite system $K_{\text{eff}}(r)$ does not renormalize to zero for temperatures in the range $T_{\text{KT}} < T < T_{\text{C}}(L)$. At an intermediate temperature $T^*(L)$, $K_{\text{eff}}(r)$ rapidly approaches the universal value $2/\pi$ and is essentially independent of r for lengths of order L. Above T^*, K_{eff} varies with r over length scales of order L, and at $T_{\text{C}}(L)$ $K_{\text{eff}}(L) = 0$.

In the region of T_{C}, $\langle M \rangle^2$ no longer depends on a single value of K_{eff} either and one could, in principle, derive an accurate expression for it by calculating $K_{\text{eff}}(q)$, then summing over spin wave modes. However, as the sum is dominated by contributions at long wavelength we approximate by writing $\langle M \rangle^2 = \exp\left(-K_{\text{eff}}^{-1}(L)G(0)\right)$. This is an excellent approximation up to $T^*(L)$, and is reasonable even at $T_{\text{C}}(L)$ where $K_{\text{eff}}(r)$ varies over the whole range from $r = 0$ to L. It then gives us an expression for χ in terms of $K_{\text{eff}}(r)$.

We indeed obtain a peak in $\chi(T)$ of approximately the correct shape, but with amplitude off by a scale factor of O(1). Rescaling the peak we obtain the fit shown in figure 7. In the region of T^* the curve fits the data very well. It is insensitive to the details of the renormalization, with different procedures simply changing the amplitude. In the region of T_{C} errors arise mainly from the fact that our calculated $K_{\text{eff}}(L)$ falls to zero at T_{C}, driving our approximate expression for $\langle M \rangle$ prematurely to zero. The position of the peak is slightly shifted to lower temperature because of this and χ is underestimated above T_{C}, where the finite-size magnetization remains, in reality non-zero. The curve shown is for renormalization by four discrete steps. In a more sophisticated theory one should take into account the discrete lattice structure. The fit, however, confirms our interpretation of the susceptibility peak: it arises from the dependence of K_{eff} on length. Physically this is a consequence of the fact that above $T \approx T^*$ the vortex distribution does not renormalize in a self-similar manner.

Our observation of a peak in the susceptibility is consistent with the recent experimental results of Elmers *et al* [24], who studied the XY-like ultrathin magnetic film Fe(100) on W(100). We defer a detailed comparison of this with other experiments, together with a more accurate calculation of the susceptibility, to a future publication.

4. Conclusion

In conclusion we have studied the fluctuations of the finite-size magnetization in the 2D XY model. We find that there is a topological difference between the distributions in the high- and low-temperature phases, even in the limit as $N \to \infty$, despite the fact that no true symmetry breaking occurs. This gives the result that, although $\langle M(N \to \infty)\rangle = 0$, the probability, $P(M_x = 0, M_y = 0)$, at the origin of the distribution is limitingly small at low temperature, and is independent of system size. We have calculated an upper bound for the value of $P(0, 0)$, equation (12), and find that it is extremely small and independent of system size N. The distribution changes to the high-temperature form as one passes through the Kosterlitz–Thouless–Berezinskii phase transition.

The fact that the variance of the distribution, $P(M_x, M_y)$ is small is nevertheless consistent with a divergent susceptibility at all temperatures below T_{KT}. We have shown that the susceptibility for a system of size N has considerable structure. In fact, it has a double divergence: the first is due to the critical nature of the low-temperature spin wave regime, and the second, occurring in addition to the first, as one passes through T_{KT}, is due to the unbinding transition of the Coulomb gas of vortex pairs.

We have shown that the distribution function for the finite-size magnetization falls onto a universal curve of the form $Q(y - \overline{y})$, $y = JT^{-1}ML^{T/4\pi}$. One might anticipate this behaviour following the general results of finite-size scaling at a critical point. However, we find a unique universal function for the entire line of critical points in the low-temperature phase of the 2D XY model, with the reduced variable y depending on two parameters L and T. There seems no reason, in general, to expect the same scaling function for critical points belonging to different universality classes and it will be interesting in the future to study the form of $P_L(M)$ for different models.

Finally we note that, as shown in the appendix the spin wave approximation for the 2D XY model is exactly soluble, which means that, in principle we could calculate all the moments of the distribution from which we should be able to reconstruct $Q(M)$.

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Appendix. Spin wave approximation

A.1. Free energy

At low temperatures one only needs to take into account the quadratic terms in the Hamiltonian (1)

$$H \approx \tfrac{1}{2} \sum_{\langle r,r'\rangle} (\theta_r - \theta_{r'})^2 \qquad \text{(A.1)}$$

where r is the position on the lattice of spin i.

The Hamiltonian is diagonalized in Fourier space:

$$H = \sum_q |\varphi_q|^2 \times \gamma_q \qquad \text{(A.2)}$$

where

$$\theta_r = \frac{1}{\sqrt{N}} \sum_q \mathrm{e}^{-\mathrm{i}qr} \varphi_q \qquad \varphi_q = \frac{1}{\sqrt{N}} \sum_r \mathrm{e}^{\mathrm{i}qr} \theta_r$$

and where, in two and three dimensions:

$$\begin{aligned} \gamma_q^{2D} &= 4 - 2\cos(q_x) - 2\cos(q_y) \\ \gamma_q^{3D} &= 6 - 2\cos(q_x) - 2\cos(q_y) - 2\cos(q_z) \end{aligned} \tag{A.3}$$

where q_{x_i} is the component of q along x_i and the lattice constant is taken to be unity. The partition function can be written in the separable form

$$Z(T) = \prod_q Z_q(T) = \prod_q \int \frac{\mathrm{d}\varphi_q}{2\pi\sqrt{N}} \exp\left(-\frac{K}{2} \sum_q |\varphi_q|^2 \times \gamma_q \right). \tag{A.4}$$

As $\gamma_0 = 0$ the Goldstone mode can be treated separately

$$Z_0 = \int_{-\pi\sqrt{N}}^{\pi\sqrt{N}} \mathrm{d}\varphi_0/(2\pi\sqrt{N}) = 1.$$

For the rest of the Brillouin zone the limits of integration are set to infinity, which is an excellent approximation at low temperature, giving

$$Z_q(T) = \sqrt{\frac{T}{2\pi J \gamma_q}} \tag{A.5}$$

and for the free energy

$$F(T) = \frac{T}{2J} \sum_{q \neq 0} \ln\left(\frac{2\pi J \gamma_q}{T} \right). \tag{A.6}$$

A.2. Green's functions and the magnetization

We work in the reference frame of the instantaneous magnetization direction

$$\bar{\theta} = \tan^{-1}\left(\frac{\sum_r \sin\theta_r}{\sum_r \cos\theta_r} \right)$$

and define the angle $\psi_r = \theta_r - \bar{\theta}$. Working in this reference frame conveniently removes the Goldstone mode from the calculation. The Green's function propagator is given by

$$\frac{T}{J} \times G(r) = \langle \psi_0 \psi_r \rangle = \frac{1}{N} \sum_{q,q'} \mathrm{e}^{-\mathrm{i}qr} \langle \psi_q \psi_{q'} \rangle. \tag{A.7}$$

Using the property $\psi_q = \varphi_q(1 - \delta(q))$, one can write:

$$\begin{aligned} \frac{T}{J} G(r) &= \frac{1}{N} \sum_{q \neq 0} \mathrm{e}^{-\mathrm{i}qr} \langle |\varphi_q|^2 \rangle \\ G(r) &= \frac{1}{N} \sum_{q \neq 0} \frac{\mathrm{e}^{-\mathrm{i}qr}}{\gamma_q}. \end{aligned} \tag{A.8}$$

The instantaneous magnetization, equation (3), can be written

$$M = \frac{1}{N} \sum_r \cos(\theta_r - \bar{\theta}) = \frac{1}{N} \sum_r \cos(\psi_r).$$

This definition of M differs from that of equation (4) by terms of higher order in $(1/N)$, which, to an excellent approximation we can neglect. The thermal average magnetization $\langle M\rangle$ is then

$$\langle M\rangle = \langle\cos(\psi_0)\rangle = \sum_{p=0}^{\infty}\frac{(-1)^p}{(2p)!}\langle\psi_0^{2p}\rangle \tag{A.9}$$

where ψ_0 represents the orientation of an arbitrary spin. As the problem is Gaussian we can apply Wick's theorem [25]:

$$\langle\psi_0^{2p}\rangle = (2p-1)!! \times \langle\psi_0^2\rangle^p = (2p-1)!! \times \left[\frac{T}{J}G(0)\right]^p \tag{A.10}$$

with $(2p-1)!! = (2p-1)\times(2p-3)\ldots\times 5\times 3$, from which we can explicitly calculate the magnetization as a function of $G(0)$

$$\begin{aligned}\langle M\rangle &= \sum_{p=0}^{\infty}\frac{(2p-1)!!}{(2p)!}\left[-\frac{T}{J}G(0)\right]^p\\ \langle M\rangle &= \sum_{p=0}^{\infty}\frac{1}{2^p\times p!}\left[-\frac{T}{J}G(0)\right]^p\\ \langle M\rangle &= \exp\left(-\frac{TG(0)}{2J}\right).\end{aligned} \tag{A.11}$$

For $D = 2$, $G_{2D}(0) = \ln(2N)/4\pi + o(N^{-1})$; the magnetization is non-intensive.

For $D = 3$, $G_{3D}(0) = a - b\times N^{-1/3} + o(N^{-1})$ with $a = 0.252\,73$, $b = 0.225\,65$; the magnetization is intensive for $N \gg 1$.

A.3. Correlation function and magnetic susceptibility

We define the pair correlation function

$$g(r) = \langle \boldsymbol{S}_0\boldsymbol{S}_r\rangle = \langle\cos(\psi_0)\cos(\psi_r)\rangle + \langle\sin(\psi_0)\sin(\psi_r)\rangle. \tag{A.12}$$

By symmetry the sum over all $\boldsymbol{r}$ of the second term is zero and it therefore does not contribute to the susceptibility, however the individual terms are not zero and contribute to $g(r)$.

Expanding the first term

$$\langle\cos(\psi_0)\cos(\psi_r)\rangle = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\frac{(-1)^{p+q}}{(2p)!\times(2q)!)}\langle\psi_0^{2p}\psi_r^{2q}\rangle \tag{A.13}$$

again using Wick's theorem, and defining $x = \langle\psi_0\psi_0\rangle$ and $y(r) = \langle\psi_0\psi_r\rangle$, we find

$$\langle\psi_0^{2p}\psi_r^{2q}\rangle = \sum_{k=0}^{\min(p,q)} y(r)^{2k}\times x^{p+q-2k}\times B(p,q,k) \tag{A.14}$$

with

$$\begin{aligned}B(p,q,k) &= \frac{(2p)!}{(2p-2k)!}\times\frac{(2q)!}{(2q-2k)!}\times\frac{1}{(2k)!}\times(2p-2k-1)!!\times(2q-2k-1)!!\\ &= \frac{(2p)!\times(2q)!}{2^{p+q-2k}\times(p-k)!\times(q-k)!}.\end{aligned}$$

Putting this into equation (A.13)

$$\langle\cos(\psi_0)\cos(\psi_r)\rangle = \sum_{k=0}^{\infty}\sum_{p=k}^{\infty}\sum_{q=k}^{\infty}\frac{1}{(p-k)!\times(q-k)!\times(2k)!}\times y(r)^{2k}\times\left(-\frac{x}{2}\right)^{p+q-2k}$$

$$= \sum_{k=0}^{\infty}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}\sum_{r}\frac{1}{p!\times q!\times(2k)!}\times y(r)^{2k}\times\left(-\frac{x}{2}\right)^{p+q}$$

$$= \left(\sum_{k=0}^{\infty}\sum_{r}\frac{y(r)^{2k}}{(2k)!}\right)\times\left(\sum_{p=0}^{\infty}\frac{1}{p!}\times\left(-\frac{x}{2}\right)^{p}\right)^{2}. \quad \text{(A.15)}$$

Using the definitions $\langle M\rangle = \exp(-x/2)$ and $y(r) = (T/J)\times G(r)$, we finally find

$$\langle\cos(\psi_0)\cos(\psi_r)\rangle = \langle M\rangle^2\cosh\left(\frac{T}{J}\times G(r)\right). \quad \text{(A.16)}$$

Following a similar analysis for the second term in equation (A.12)

$$\langle\sin(\psi_0)\sin(\psi_r)\rangle = \langle M\rangle^2\sinh\left(\frac{T}{J}\times G(r)\right)$$

from which we find

$$g(r) = \langle M\rangle^2\exp\left(\frac{T}{J}\times G(r)\right). \quad \text{(A.17)}$$

Summing over $g(r)$ one finds the second moment of the distribution $Q(M)$

$$\langle M^2\rangle = \frac{1}{N}\sum_{r} g(r) \quad \text{(A.18)}$$

which, from equation (5), gives for the susceptibility per spin

$$\chi = \frac{\langle M\rangle^2}{T}\sum_{r}\left[\exp\left(\frac{T}{J}\times G(r)\right)-1\right]. \quad \text{(A.19)}$$

At low temperatures we can expand the exponential

$$\chi \simeq \frac{T\langle M\rangle^2}{2J^2}\sum_{r}G(r)^2 = \frac{T\langle M\rangle^2}{2JN^2}\sum_{r}\sum_{q\neq 0}\sum_{q'\neq 0}\frac{\mathrm{e}^{\mathrm{i}(q+q')r}}{\gamma_q}$$

and finally we have

$$\chi \simeq \frac{T\langle M\rangle^2}{2J^2}A(N) \qquad \text{with } A(N) = \frac{1}{N}\sum_{q\neq 0}\left(\frac{1}{\gamma_q}\right)^2. \quad \text{(A.20)}$$

Using a continuum approximation it is easy to see that $A_{2D}(N)$ is proportional to N, while $A_{3D}(N)$ varies as $N^{1/3}$. A numerical sum over the N particle Brillouin zone gives:

- for two dimensions, $A_{2D}(N) = N/a_{2D}$, with $a_{2D} = 258.59$;
- for three dimensions, $A_{3D}(N) = N^{1/3}/a_{3D}$, with $a_{3D} = 93.606$.

We remark therefore that in three dimensions the susceptibility per spin remains weakly divergent despite the establishment of true long-range magnetic order at low temperature. This is because the density of spin wave states at small wave vector is sufficiently high to produce anomalous fluctuations, although in this case the bulk magnetization is not destroyed and it is not a critical effect, as discussed in the main text. From (A.20) one can see that χ becomes intensive only in four dimensions.

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