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LETTER TO THE EDITOR

Phase transitions in the classical XY antiferromagnet on the triangular lattice

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Abstract. The critical behaviour of the fully frustrated classical antiferromagnet on the triangular lattice is studied using Monte Carlo methods. Numerical evidence for separate Kosterlitz–Thouless and Ising transitions is presented as a result of investigating the free-energy cost to create an isolated vortex, the finite-size scaling of the spin stiffness and the finite-size scaling of the chirality.

Frustrated two-dimensional XY models have attracted much attention recently. Studies of phase transitions in these models are motivated by their relevance to systems such as arrays of Josephson junctions in an applied magnetic field [1], helimagnets [2, 3] and discotic liquid crystals [4]. The fully frustrated XY model (FFXY) has a ground state with continuous $U(1)$ and discrete Z_2 symmetry. The discrete Z_2 symmetry implies that an Ising-type transition occurs at a temperature T_{I} while the continuous $U(1)$ symmetry should give rise to a Kosterlitz–Thouless (KT) [5] vortex unbinding transition at T_{KT}. The simplest example of a fully frustrated XY system is the classical antiferromagnet on a triangular lattice. The ground state of the system is a non-collinear spin arrangement in which the spins on each triangle make an angle of 120° with one another. There are two distinct arrangements depending on the sense of rotation of the spins around each triangle, and each is characterized by a left or right chirality. The Ising symmetry arises due to the two chiralities of the ground state. It is expected that T_{I} is higher than T_{KT}, but a single transition with exponents in a different universality class cannot be ruled out.

Several Monte Carlo simulations [6–9] have been reported for the FFXY model on the triangular and square lattice. However, no definite conclusions on the critical behaviour have been reached. Early simulations [7] for the triangular lattice suggested a double transition with $T_{\mathrm{I}} > T_{\mathrm{KT}}$, and the critical exponents associated with the Ising order parameter (the chirality) were found to be consistent with the pure ($d = 2$) Ising values. Mean-field calculations [10] as well as renormalization-group calculations [11, 12] support the idea of a single transition with $T_{\mathrm{I}} = T_{\mathrm{KT}}$. Recent Monte Carlo simulations [13–16] also suggest a single transition which belongs to a new universality class. The authors argue that previous numerical evidence for an Ising-type transition was mainly drawn from the finite-size scaling of the specific heat and is unreliable. The evidence for a single transition, however, is not conclusive. Other studies on the square lattice [17, 18] find evidence for two transitions but with scaling behaviour different from that expected for the KT and Ising transitions.

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In this letter, we report detailed Monte Carlo simulations for the FFXY model on the triangular lattice. We provide numerical evidence for two phase transitions: a KT phase transition at a temperature below that corresponding to the appearance of the chirality order parameter. A similar conclusion for the square lattice has recently been reported by Olsson [19]. We define and calculate a vorticity modulus which measures the free-energy cost to create an isolated vortex. This provides *direct* evidence for a Kosterlitz–Thouless vortex binding–unbinding phase transition in this model. We also perform a finite-size scaling analysis of the spin stiffness, and the quality of the fit to the KT finite-size scaling form allows us to locate the KT transition temperature to an accuracy of less than 1%. Finally, we investigate the finite-size scaling behaviour of the chirality and show that the transition temperature for the chiral order is higher than that of the KT transition.

The classical XY model with nearest-neighbour interactions is described by the Hamiltonian

$$H = J\sum_{i<j} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

where $\boldsymbol{S}_i$ represents a classical 2-component spin of unit magnitude, located at the sites of a triangular lattice. In the present case, positive J corresponds to the FFXY model. The ferromagnetic XY model has a Kosterlitz–Thouless phase transition [20, 21] at a finite temperature where vortices unbind. The transition is accompanied by an abrupt change in the spin stiffness, or helicity modulus. The classical ground state of the FFXY model on the triangular lattice has the spins oriented at 120° to one another. This order corresponds to one of the two inequivalent reciprocal lattice vectors $\boldsymbol{Q} = (\pm\frac{4\pi}{3}, 0)$. These two chiralities are topologically distinct in the XY model since no continuous transformation can transform one ground-state configuration into the other. This discrete degeneracy combined with continuous rotational spin symmetry provides a rich critical behaviour for the FFXY model.

One way to unambiguously identify a defect-mediated phase transition is to calculate the excess free energy of a free vortex. According to the original KT argument [5], this excess energy is zero for $T > T_{\mathrm{KT}}$ and positive for $T < T_{\mathrm{KT}}$. Kawamura and Kikuchi [22] have proposed a method to measure this energy difference using Monte Carlo simulations with two different sets of boundary conditions. The free-energy difference gives an estimate of the excess free energy of a single free vortex. More recently, Southern and Xu [23] have introduced a quantity called vorticity to directly measure the free-energy cost to create an isolated vortex in the frustrated Heisenberg model on the triangular lattice. This response function has the advantage that it can be calculated using the usual periodic boundary conditions.

The spin stiffness [24], or helicity modulus, is a measure of the response of the spin system to a twist over the length of the lattice and can be calculated using the expression [23]

$$\rho(L) = -\frac{J}{L^2}\sum_{i<j}(\hat{e}_{ij}\cdot\hat{\boldsymbol{u}})^2\langle S_i^x S_j^x + S_i^y S_j^y\rangle - \frac{J^2}{L^2 T}\left\langle\left(\sum_{i<j}(\hat{e}_{ij}\cdot\hat{\boldsymbol{u}})[S_i^x S_j^y - S_i^y S_j^x]\right)^2\right\rangle \tag{2}$$

where $\hat{e}_{ij}$ are unit vectors along neighbouring bonds and $\hat{\boldsymbol{u}}$ is the *direction* of the twist *in the lattice*. In a similar manner, a vorticity can be defined as the response of the spin system to an imposed twist about an axis perpendicular to the spin plane along a closed path which encloses a vortex core. This is essentially the response of the system to an isolated vortex and can be calculated as the second derivative of the free energy with respect to the strength of the vortex, or winding number m, evaluated at $m = 0$. We obtain the following expression for the XY model:

$$V(L) = \frac{-2J}{\sqrt{3}} \sum_{i<j} \left(\frac{\hat{e}_{ij} \cdot \hat{\phi}_{\mathbf{i}}}{r_i} \right)^2 \langle S_i^x S_j^x + S_i^y S_j^y \rangle - \frac{2J^2}{\sqrt{3}T} \left\langle \left(\sum_{i<j} \left(\frac{\hat{e}_{ij} \cdot \hat{\phi}_{\mathbf{i}}}{r_i} \right) [S_i^x S_j^y - S_i^y S_j^x] \right)^2 \right\rangle \tag{3}$$

where we have arbitrarily chosen the origin of the vortex to be at the centre of one of the triangles near the middle of the lattice. The positions of the spins are specified using polar coordinates (r_i, ϕ_i) relative to this point. Hence r_i is the distance of site i from the vortex core and $\hat{\phi}_i$ is tangential to the circular *path in the lattice* passing through site i and enclosing the vortex. The vorticity has been normalized by the unit cell area. Here, V contains both a core contribution and a part which is proportional to $\ln(L/a)$. By comparing different lattice sizes, L, we can extract the vorticity modulus v defined as follows:

$$V(L) = C + v \ln(L/a) . \tag{4}$$

To calculate the vorticity we have performed Monte Carlo (MC) simulations on lattices of linear sizes, $L = 12, 24, 36, 48, 72, 96, 144$, using a Metropolis algorithm with over relaxation [25, 26]. The first combined 1.4×10^5 MC sweeps are discarded and the next 5.6×10^5 combined MC sweeps are used to calculate V. A typical run of size $L = 96$ requires about 36 CPU hours on an IBM RS6000 workstation.

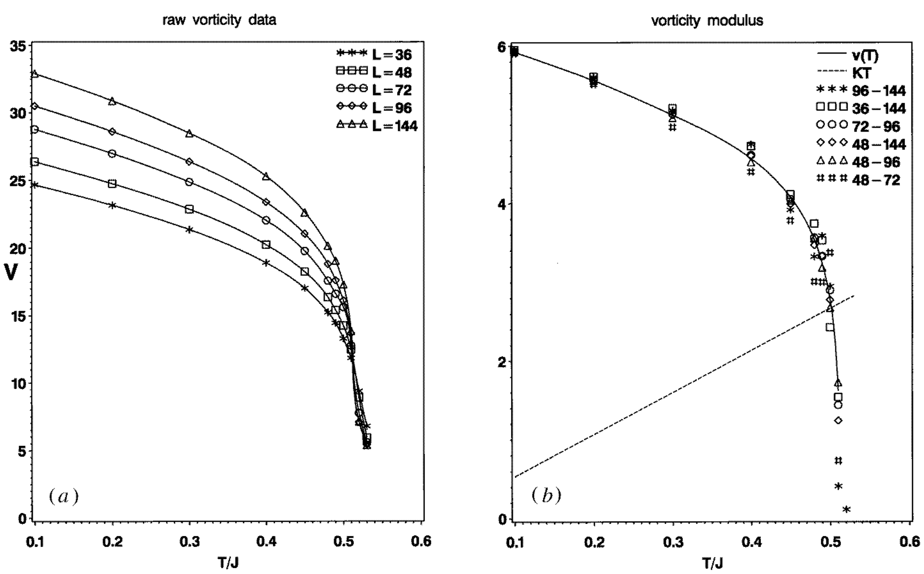

Figure 1. (a) Raw data for the vorticity $V(L)$, as a function of T/J, obtained from equation (3) using different system sizes L. (b) The vorticity modulus $v(T)$, as a function of T/J, obtained from equation (4) by comparing systems of different sizes is shown by the symbols. The full curve is an average over all pairs. The broken curve represents the universal jump $v(T)/v(0) = \frac{8}{3\pi} T/J$ predicted by the KT theory.

Figure 1(a) shows the raw data for $V(L)$ for various sizes and figure 1(b) shows the vorticity modulus v as a function of T/J, obtained by comparing sizes L_1 and L_2. Apart from finite-size effects, we clearly see that the vorticity goes to zero for $T > 0.51J$. Our numerical data indicates that at high temperatures there is no energy cost to create a free vortex, while for lower temperatures the cost is proportional to $\ln L$. We have also calculated the reduced stiffness, $\rho(T)/\rho(0)$, using equation (2) for the same lattice sizes and the results are compared to the reduced vorticity modulus, $v(T)/v(0)$, in figure 2. Our results for the vorticity and the spin stiffness show identical temperature dependences, with both quantities vanishing abruptly at the same temperature. The fact that these two response functions behave identically for the FFXY model is, presumably, due to the fact that the spin wave and vortex degrees of freedom are uncoupled, in contrast to the situation in the frustrated Heisenberg case [23]. Using the KT value [27] of the reduced stiffness at the transition, $\rho(T)/\rho(0) = \frac{8}{3\pi}T/J$, we estimate that $T_{\mathrm{KT}} \sim 0.50J$.

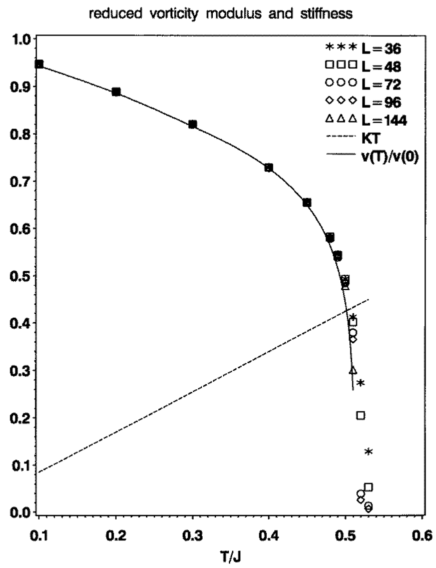

Figure 2. The full curve represents the reduced vorticity modulus, $v(T)/v(0)$, and the symbols represent the reduced spin stiffness, $\rho(T)/\rho(0)$, for various sizes, L, as a function of T/J. The broken line represents the predictions of the Kosterlitz–Thouless (KT) theory.

Weber and Minnhagen [28] were able to locate T_{KT} for a two-dimensional ferromagnetic XY model to a few tenths of a per cent, using the finite-size scaling form of the spin stiffness at the KT transition temperature. At the transition the reduced spin stiffness behaves as

$$\frac{\rho(L)}{\rho(0)} = \frac{8}{3\pi}\frac{T}{J}\left(1 + \frac{1}{2\ln(L/L_0)}\right) \tag{5}$$

where the parameter L_0 is a constant. We choose a value of T and fit the measured spin stiffness $\rho(L)$ to the above KT scaling form which has only the one free parameter L_0. The deviation from the fit, $\chi^{\mathrm{KT}}_{\mathrm{sq}}$, is plotted as a function of T/J in figure 3. One can easily see that $\chi^{\mathrm{KT}}_{\mathrm{sq}}$ increases significantly for T larger than $0.506J$ and smaller than $0.496J$. The position of the minimum suggests that the transition temperature is given by $T_{\mathrm{KT}} = (0.501 \pm 0.002)J$. The fact that the KT scaling form with only one adjustable parameter fits the stiffness data extremely well can be taken as strong evidence that the phase transition is of the KT type. Miyashita and Shiba [7] have previously estimated $T_{\mathrm{KT}} = (0.502 \pm 0.002)J$ using the KT exponent criterion $\eta(T) = \frac{1}{4}$. This agreement provides further evidence for a KT transition.

So far we have only discussed the $U(1)$ symmetry of the model and have provided numerical evidence of a KT transition at $T_{\mathrm{KT}} = (0.501 \pm 0.002)J$. We now show that our estimate of the transition temperature for chiral order is higher. The chirality on each elementary triangle R is defined as follows (see, for example, [7]):

$$\kappa(R) = \frac{2}{3\sqrt{3}}(\boldsymbol{S}_2 \times \boldsymbol{S}_1 + \boldsymbol{S}_3 \times \boldsymbol{S}_2 + \boldsymbol{S}_1 \times \boldsymbol{S}_3) \cdot \hat{\boldsymbol{k}} \tag{6}$$

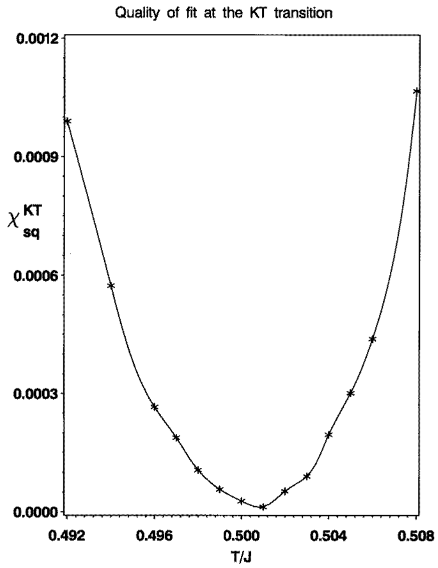

Figure 3. $\chi_{\rm sq}^{\rm KT}$ as a function of the trial value of $T_{\rm KT}$ in units of J.

where $\boldsymbol{S}_1$, $\boldsymbol{S}_2$, $\boldsymbol{S}_3$ are the three spins at the corners. The chirality is normal to the spin plane for the XY model and can take any value in the range $[-1, 1]$. In the ground state, the chirality on each triangle takes the values $+1$ or -1 and thus resembles an Ising spin. We have calculated $\langle P^2\rangle$ for various system sizes, where $P = \sum_R \kappa(R)/N_\triangle$ is the chirality order, parameter and $N_\triangle$ is the total number of triangles. The chirality appears to develop at a higher temperature than our estimate of $T_{\rm KT}$.

In order to examine the critical behaviour we have used the following finite-size scaling form [29] for the order parameter P:

$$\langle P^2\rangle = N_\triangle^x f_\pm(tN^y) \tag{7}$$

where $x = 2(\beta+\gamma)/(2\beta+\gamma)$, $y = 1/(2\beta+\gamma)$, t is the reduced temperature $t = |T - T_{\rm c}|/T_{\rm c}$ and the $\pm$ indicates the form above and below $T_{\rm c}$. Here β and γ are the usual critical exponents for the order parameter and susceptibility, respectively. For each trial value of $T_{\rm c}$, we collapse the data using a ln–ln plot of $\langle P^2\rangle/N_\triangle^x$ against tN^y to determine β and γ. The sum of the quality of fits to the two scaling forms, $\chi_{\rm sq}^{\rm I}$, is shown as the trial function $T_{\rm c}$ in figure 4. The quality of the fit deteriorates for $T < 0.506J$ and $T > 0.516J$, and from the minimum we estimate the critical transition temperature $T_{\rm c} = (0.511 \pm 0.003)J$. Note that this estimate is close to the value of $(0.513 \pm 0.002)J$ obtained by Lee *et al* [13]. Using the location of the specific heat maximum, Miyashita and Shiba [7] obtained an estimate for the chiral transition temperature equal to $0.513J$. Our data suggests that the Z_2 transition temperature is higher than $T_{\rm KT}$ and that there are two transitions in agreement with Miyashita and Shiba. Our fit of the chirality to the finite-size scaling forms yields the values $\beta = 0.11 \pm 0.03$ and $\gamma = 1.6 \pm 0.3$ for the critical exponents. These estimates do not differ significantly from the pure Ising values but the error is quite large.

In summary, we have provided numerical evidence that there are two phase transitions in the FFXY model on the triangular lattice. The Z_2 transition temperature is found to be higher than the $U(1)$ KT transition temperature. We have calculated a direct measure of the excess free energy for a free vortex. This excess free-energy vanishes at high temperatures and varies as $\ln L$ below $T_{\rm KT} = (0.501 \pm 0.002)J$. These results provide direct evidence of a vortex binding–unbinding mechanism for the phase transition. The vorticity shows the same

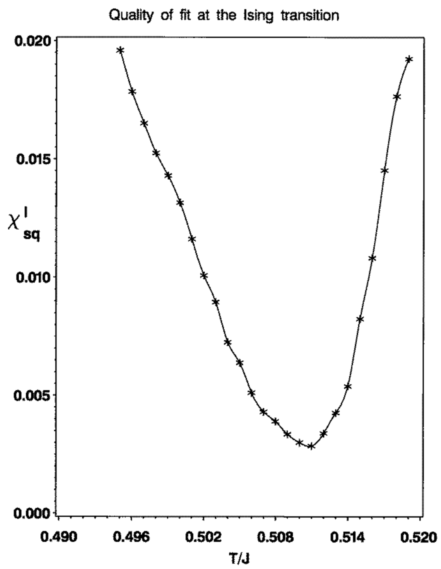

Figure 4. $\chi^{\rm I}_{\rm sq}$ as a function of the trial value of T_c in units of J.

temperature variation as the spin stiffness and both quantities vanish at T_{KT}. Furthermore, we find that a finite-size scaling analysis of the spin stiffness data fits the KT form extremely well at the critical temperature. Our results are consistent with the previous estimate of T_{KT} by Miyashita and Shiba, using the criterion $\eta = \frac{1}{4}$. On the other hand, we estimate the chiral order transition to be at a higher temperature, $T_c = (0.511 \pm 0.003) J$, with exponents which do not differ significantly from the pure Ising values. In a recent paper, Olsson [19] studied the FFXY model on the square lattice and reached the same conclusions.

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