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Monte Carlo study of the Heisenberg antiferromagnet on the triangular lattice

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We report a Monte Carlo study of the classical antiferromagnetic Heisenberg model on the triangular lattice. The free-energy cost for the formation of free vortices is obtained from a vorticity modulus. Evidence of a Kosterlitz-Thouless type of defect-mediated phase transition at a finite temperature is found.

I. INTRODUCTION

The classical Heisenberg model on the two-dimensional triangular lattice with antiferromagnetic nearest-neighbor coupling J is *frustrated*. As a result, a collinear arrangement of the spins at low temperature is not the lowest energy configuration. There is, however, an ordered ground state which has three sublattices with a *noncollinear* arrangement of the spins on each triangle. The spins lie in a plane at an angle of 120° with respect to one another corresponding to one of the two inequivalent ordering wave vectors $\mathbf{Q}=(\pm 4\pi/3,0)$. The local order parameter is similar to a rigid body with three principal axes and belongs to the SO(3) rotation group.[1,2] This enlarged symmetry of the order parameter suggests that this model belongs to a different universality class[3–6] than the corresponding model on bipartite lattices where there is no frustration and the order parameter corresponds to a unit vector.

The SO(3) symmetry of the order parameter also allows for the existence of a stable topological (vortex) defect.[1,2] These defects have an energy which is logarithmic in the size of the system at low temperatures and thus the question of whether a Kosterlitz-Thouless[7] defect unbinding transition can occur in this system at a finite temperature should be considered.

Previous work on this possibility has been inconclusive. Kawamura and Miyashita[1] first suggested the possibility of such a transition and studied relatively small system sizes using Monte Carlo methods. Their results suggested a finite temperature phase transition at $T=0.31J$ accompanied by a rapid appearance of free vortices above this temperature. Azaria *et al.*[3–5] used a continuum version of the model and employed renormalization-group (RG) techniques to study the pair-correlation length and the effective long-wavelength spin stiffness at low T. They did not include any vortex degrees of freedom in their calculations and their results suggested a phase transition at $T_c=0$ with an enlarged SO(3) symmetry. Wintel *et al.*[8] have recently studied the effect of vortex-spin wave interactions within the continuum model and they suggest that there should be a sharp crossover in the correlation length at a finite temperature. However, their results were restricted to vortex separations smaller than the spin-wave correlation length and the possibility of a true transition accompanied by the *abrupt* appearance of free vortices remains unresolved. Southern and Young[9] have also used Monte Carlo and high-temperature methods to study the model. The two-spin correlation length and the structure factor $S(\mathbf{Q})$ were calculated and both exhibited a rapid crossover in behavior at about $T=0.32J$ which may be related to the disappearance of free vortices. However, the results for the spin stiffness were in excellent agreement with the low T RG which does not predict a finite T transition.

In the present work, we study the free-energy cost of vortex formation in the system at low temperatures. We define a vorticity modulus in terms of an equilibrium correlation function. Our results indicate that a Kosterlitz-Thouless (KT) type of transition may indeed occur at a finite value of T.

II. MODEL

The Hamiltonian of the system is given by

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

where $\mathbf{S}_i$ represents a classical three-component spin of unit magnitude located at each site i of a triangular lattice of L^2 sites and the interactions are restricted to nearest-neighbor pairs. Domain-wall arguments[10] applied to both the Heisenberg ferromagnet and antiferromagnet on bipartite lattices in two dimensions indicate that there is no phase transition in this model at finite temperatures. This is due to the fact that transverse fluctuations of the order parameter destroy long-ranged order at all finite temperatures.

Information about the rigidity of the order parameter against fluctuations can be obtained from the spin-wave stiffness coefficient. The spin stiffness (helicity) tensor is given by the second derivative of the free energy[9,11] with respect to the twist angle about a particular direction in spin space. In the present case of the antiferromagnet on the triangular lattice, we choose two orthogonal directions $\hat{\mathbf{n}}_1,\hat{\mathbf{n}}_2$ in the plane of the spins and a third direction $\hat{\mathbf{n}}_3$ perpendicular to the plane. We apply a twist about each of these axes and the corresponding stiffness is given by[9]

$$\rho_\alpha=\frac{2J}{\sqrt{3}L^2}\sum_{i<j}(\hat{\mathbf{e}}_{ij}\cdot\hat{\mathbf{u}})^2\langle S_i^\beta S_j^\beta+S_i^\gamma S_j^\gamma\rangle - \frac{2J^2}{\sqrt{3}L^2T}\left\langle\left(\sum_{i<j}(\hat{\mathbf{e}}_{ij}\cdot\hat{\mathbf{u}})[S_i^\beta S_j^\gamma-S_i^\gamma S_j^\beta]\right)^2\right\rangle, \tag{2}$$

where $\alpha=1,2,3$ and α,β,γ are to be taken in cyclic order. S_i^α denotes the component of the spin at site i in the $\hat{\mathbf{n}}_\alpha$ direction, $\hat{\mathbf{e}}_{ij}$ are unit vectors along neighboring bonds, and $\hat{\mathbf{u}}$ is the *direction* of the twist *in the lattice*. All stiffnesses have been normalized by the unit-cell area. As mentioned in the previous section, a Monte Carlo method[9] has been used to calculate these stiffness coefficients at low T and the results are in excellent agreement with the two-loop RG calculations.[5] The spin stiffness of the Heisenberg antiferromagnet decreases at large length scales and there is no long-ranged sublattice order at finite temperature.

In the same way that the spin stiffness is a measure of the response of the spin system to a twist over the length of the lattice, a vorticity can be defined as the response of the spin system to an imposed twist about a given axis α in spin space 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:

$$V_\alpha=\frac{2J}{\sqrt{3}}\sum_{i<j}\left(\frac{\hat{\mathbf{e}}_{ij}\cdot\hat{\boldsymbol{\phi}}_i}{r_i}\right)^2\langle S_i^\beta S_j^\beta+S_i^\gamma S_j^\gamma\rangle - \frac{2J^2}{\sqrt{3}T}\left\langle\left[\sum_{i<j}\left(\frac{\hat{\mathbf{e}}_{ij}\cdot\hat{\boldsymbol{\phi}}_i}{r_i}\right)[S_i^\beta S_j^\gamma - S_i^\gamma S_j^\beta]\right]^2\right\rangle, \quad (3)$$

where r_i is the distance of site i from the vortex core and $\hat{\boldsymbol{\phi}}_i$ is tangent to the circular *path in the lattice* passing through the site i and enclosing the vortex. Here α,β,γ are defined in the same way as for the stiffnesses and indicate the axis of rotation of the vortex.

The V_α contain 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_α defined as follows:

$$V_\alpha=C_\alpha+v_\alpha\ln(L/a). \quad (4)$$

Kawamura and Kikuchi[12] have also recently calculated a vorticity modulus for two ferromagnetic models. They calculate the free energies for different boundary conditions and subtract them to obtain the part which varies as $\ln(L/a)$. Our approach does not require any change in boundary conditions and is applied directly to the antiferromagnetic model.

III. RESULTS

In this section we describe our Monte Carlo results for the vorticity of the Heisenberg antiferromagnet. We have used a single spin-flip heat bath algorithm[13] to update the spin directions at each Monte Carlo step and all thermal averages are replaced by time averages. For the largest value of the system size $L=192$ studied we discard the first 10^4 steps and perform averages over the next 10^5 steps. Figure 1 shows the raw data obtained for the average of the three vorticities, $V=\Sigma_{\alpha=1}^3 V_\alpha/3$, as a function of T/J for various system sizes L. At low T, the free-energy cost for creating isolated vortices increases logarithmically with L but, as T increases, the curves all appear to cross at a unique value of the temperature near $T\sim 0.305\pm 0.005J$. The behavior suggests that an abrupt change in the rigidity of the system against the formation of isolated vortices occurs at this temperature.

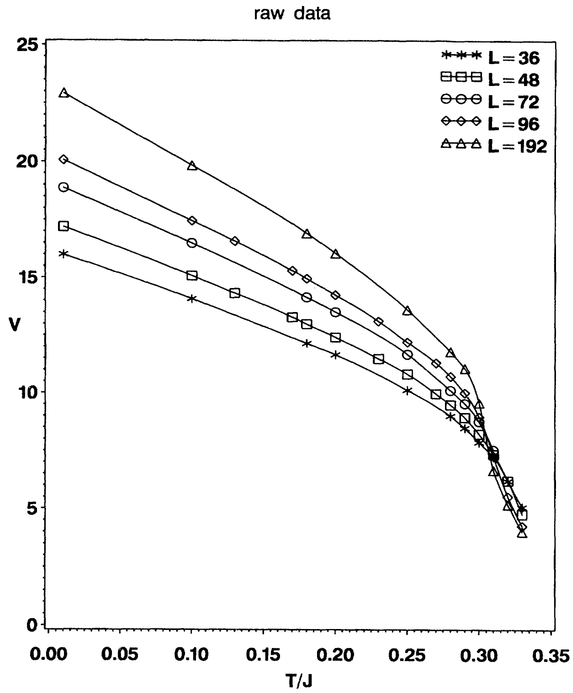

FIG. 1. Raw data obtained using Eq. (3) for the average of the three vorticities for different system sizes L as a function of T/J.

The raw data contains a contribution which is independent of the size of the system as well as a contribution proportional to $\ln L$. The size independent part is a vortex core contribution and the coefficient of the $\ln L$ term is defined to be the vorticity modulus and can be obtained by using the results obtained for systems of size L_1 and L_2 as follows:

$$v_\alpha=\frac{V_\alpha(L_2)-V_\alpha(L_1)}{\ln(L_2/L_1)}. \quad (5)$$

Figure 2 shows the vorticity moduli v_α obtained using the method above for various choices of system sizes L_1,L_2 plotted as a function of T/J. At zero temperature, the moduli approach the values $v_3=2\pi$, $v_1=v_2=\pi$ and all decrease as T increases until about $T\sim 0.3J$ where they all become equal and then abruptly drop to zero. Kawamura and Miyashita[1] identified two basic types of vortices for this model and our results suggest that both types of vortex become free at the same temperature.

The average of the three vorticity moduli, $v(T)$, obtained from comparing different sizes is shown in Fig. 3 as a function of T/J. A naive application of the Kosterlitz-Thouless[7] theory of vortex unbinding would predict that a transition occurs when the following line[14]

$$\frac{v(T)}{v(0)}=\frac{8}{3\pi}\frac{T}{J} \quad (6)$$

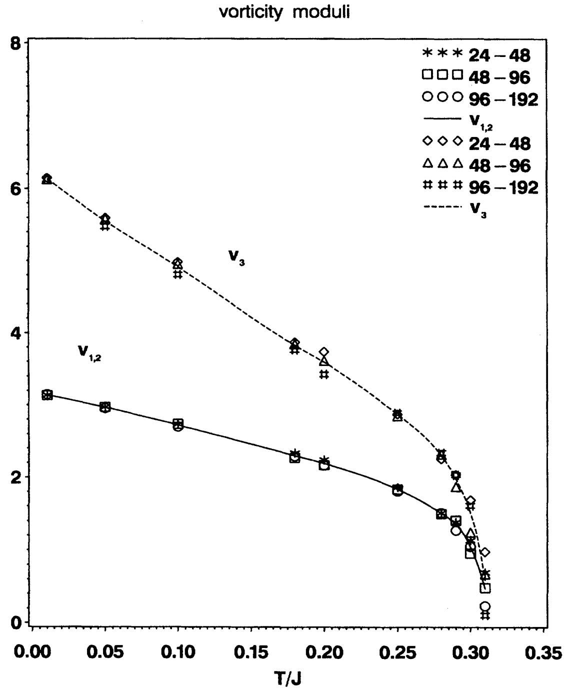

FIG. 2. The vorticity moduli as a function of T/J obtained by comparing systems of different size.

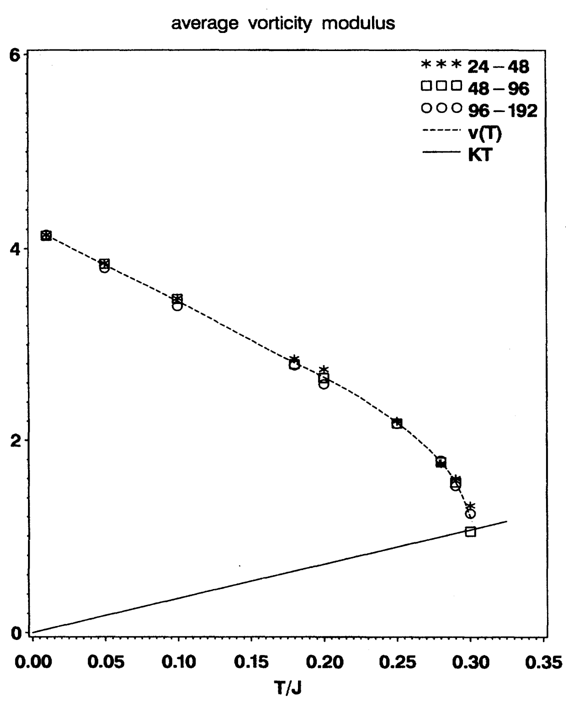

FIG. 3. The dashed curve and symbols represent the average of the three vorticity moduli as a function of T/J. The solid line represents the predictions of the Kosterlitz-Thouless (KT) theory.

intersects the calculated (renormalized) vorticity. This relation would describe the universal jump in the vorticity at the transition if it behaves in the same way as the spin stiffness in the XY model on the triangular lattice. This line is represented by the solid curve in Fig. 3 and the two curves intersect at about $T=0.305\pm0.005J$. The results suggest that a KT type of transition may indeed occur in the Heisenberg antiferromagnet and that it belongs to the XY universality class. However, the details of the transition differ from the XY model in that the vorticity has a jump but the spin stiffness does not. Hence it appears that we must distinguish between these two quantities in the Heisenberg antiferromagnet. We have also calculated[15] both the spin stiffness (helicity) and vorticity as defined above for the ferromagnetic XY model on this same lattice. In this case, both quantities behave identically and *both* exhibit a jump at the same finite value of T.

IV. SUMMARY

The Heisenberg antiferromagnet on the triangular lattice is frustrated and the preferred arrangement of the spins is in a plane at $T=0$. The corresponding order parameter is noncollinear and the symmetry allows for the existence of topological defects. Previous Monte Carlo calculations found an extremely rapid crossover in the behavior of the antiferromagnetic structure factor and the corresponding correlation length near $T=0.32J$ which may be related to the disappearance of free vortices of the type identified by Kawamura and Miyashita.[1] However, results for the spin stiffnesses at low T obtained in the same calculations were in excellent agreement with the predictions[3–5] of the nonlinear sigma model which neglects vortices and predicts $T_c=0$. The previous work[9] indicated that the spin stiffness vanishes at large length scales and that the two-spin correlation length is finite at all nonzero T but that there is a transition at $T_c=0$ with an enlarged symmetry.

In the present work, the same numerical approach was used to calculate the rigidity of the system against the formation of free vortices at low temperatures. The vorticity stiffness is finite at low T and disappears abruptly near $T=0.31J$. The behavior is consistent with a defect unbinding transition of the Kosterlitz-Thouless type except that the vorticity and spin stiffness behave differently. The spin stiffness is zero on large length scales at all finite temperatures but the vorticity exhibits a jump at a finite value of T. The rapid crossover in the structure factor and two-spin correlation length reported previously[9] indicates that the spin wave and vortex degrees of freedom are strongly coupled in this model. In the Kosterlitz-Thouless theory of defect unbinding, the spin wave and vortex degrees of freedom are uncoupled at low T. A proper theoretical description of the Heisenberg antiferromagnet must take account of the interactions between vortices and spin waves.

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[14]A factor of 3/2 must be introduced into J to account for the larger coordination of the triangular lattice compared to the square lattice as well as a factor of 1/2 for the antiferromagnetic correlations.
[15]Details will be presented in a separate publication.