Frustrated Heisenberg Antiferromagnets between $d = 2$ and $d = 3$

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(Dated: March 22, 2022)

The anitiferromagnetic Heisenberg model on a stacked triangular geometry with a finite number of layers is studied using Monte Carlo methods. A topological phase transition occurs at finite temperature for all film thicknesses. Our results indicate that topological excitations are important for a complete understanding of the critical properties of the model between two and three dimensions.

PACS numbers: 75.10.Hk, 75.40.Cx, 75.40.Mg

The behavior of the Heisenberg antiferromagnet on triangular geometries is quite unusual. The ground state order parameter has SO(3) symmetry which allows for a $Z_2$ topological defect. In $d = 2$, there is a finite temperature vortex unbinding transition which is purely topological in character. Both above and below this temperature the spin-spin correlation function decays exponentially with distance. This behavior is quite different from the Kosterlitz-Thouless transition which occurs in two-dimensional $XY$ models. In the latter case the correlations are exponential at high $T$ and decay with a power law at all temperatures below the transition. There is no long range order but there is a finite spin wave stiffness in the low temperature phase. In the Heisenberg antiferromagnet, both the sublattice magnetizations and the spin wave stiffness are zero at all finite temperatures. On the other hand the vorticity modulus is nonzero at low $T$ and drops to zero at the transition. Hence the phase transition is similar to the Kosterlitz-Thouless transition in that vortices are involved but it is different in that the correlations decay exponentially at all finite temperatures.

Field theoretic studies of this model in terms of the nonlinear sigma model ($NL\sigma$) predict that there is only a transition at $T_c = 0$ in two dimensions. However a fixed-dimension perturbative approach\cite{1,2,3,4,5} in $d = 2$ using the corresponding Landau-Ginzburg-Wilson (LGW) Hamiltonian has located a fixed point which may describe a topological phase transition. In $d = 3$ both theory and experiment indicate that there is a conventional phase transition with the appearance of an order parameter below the critical temperature. However there is a great deal of debate about the nature of this transition. Monte Carlo studies and perturbative field theory calculations in fixed dimension\cite{1} indicate a continuous transition which belongs to a new chiral universality class whereas non-perturbative RG (NPRG) studies indicate a phase transition which is very weakly first order with effective exponents\cite{1,2,3}. A very recent numerical study of the RG flow in the LGW Hamiltonian by Itakura\cite{1} also suggests a possible weak first order transition for the Heisenberg spin model but with much stronger evidence for a first order transition in the case of $XY$ spins\cite{1,2}. The experimental studies of these three dimensional stacked triangular systems find that they exhibit a continuous phase transition with a set of critical exponents that do not belong to any of known universality classes.

In this work we explore the crossover of the $d = 2$ behavior to $d = 3$. We study the nature of the ordering process of a layered triangular system having dimensions $L \times L \times H$ with the number of stacked triangular layers ranging from $H = 2$ to $H = 24$ and the linear size of each layer $L$ ranging from 18 to 120 by means of Monte Carlo simulations.

We consider an isotropic Heisenberg model of classical spins interacting via nearest neighbour exchange on a layered triangular lattice described by the following Hamiltonian

$$H = - \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

Within each triangular layer the spins interact antiferromagnetically $J_{ij} < 0$. Between adjacent layers the interaction can be taken to be positive or negative with no essential difference since there is no frustration associated with these interactions and hence there is a symmetry with respect to the sign. We shall choose it to be ferromagnetic $J_{ij} > 0$ and set $|J_{ij}| = J = 1$ for all interactions. Periodic boundary conditions are applied in the plane of each triangular layer where, in order to preserve the 3-sublattice structure, it is important to choose $L$ to be a multiple of 3. The finite layer thickness, $H$, can have any integer value since we have chosen the inter-planar interactions to be ferromagnetic. The top and bottom surface layers are subject to free boundary conditions.

The spin stiffness\cite{1,2,3}, or helicity modulus, is a measure of the increase in free energy associated with a twisting of the order parameter in spin space by imposing a gradient of the twist angle about some axis $\hat{n}$ in spin space along some direction $\hat{u}$ in the lattice. Diagonal elements of the spin wave stiffness tensor can be calculated by choosing an orthogonal triad for the directions of three principal axis in spin space. The symmetry of the ground state suggests that two of the principal axes correspond to two perpendicular directions $\perp_1$ and $\perp_2$.
in the spin plane and that the third is perpendicular to this plane. This third axis is conveniently chosen to point along the average chirality direction $\hat{K}$.

Another quantity of interest when topological properties of the system are to be considered is the vorticity $V$.

The vorticity is a measure of the response of the spin system to an imposed twist about a given axis $\hat{n}$ in spin space along a closed path that encloses a vortex core. The vorticity $V_{\hat{n}}$ contains a contribution due to the vortex core as well as part which is proportional to $\ln(L/a)$. This can be written as

$$V_{\hat{n}} = C_{\hat{n}} + v_{\hat{n}} \ln(L/a).$$

where $C_{\hat{n}}$ is a temperature dependent constant describing the core and $v_{\hat{n}}$ is called the the vorticity modulus. It plays a similar role to the spin stiffness and vanishes at a phase transition.

Azaria et al. have made detailed predictions for the dependence of the stiffnesses on the linear size of the system for single layers based on the continuum limit of this model. Their results for a nonlinear sigma model (NL$\sigma$) using renormalization group (RG) techniques showed that the spin wave stiffness of the triangular antiferromagnet is a nontrivial function of $\ln L$ at low temperatures where $L$ is the linear dimension of the triangular lattice. At any finite temperature $T$, the stiffnesses are zero on length scales large compared with the correlation length. However, on length scales $1 \ll L \ll \xi$, the stiffnesses are nonvanishing at low $T$.

In order to make a comparison of our calculated stiffnesses with the predictions of the RG equations, we first calculate the stiffnesses for linear size $L = 18$ so that the condition $H \ll L$ is satisfied. Using the values at this length scale, we numerically integrate the expressions of Azaria et. al. with these initial values to predict the behavior at larger length scales. We then compare the predicted curves with the values obtained directly using Monte Carlo methods at the relatively low temperature $T = 0.2$ for different layer thicknesses. The dependence of the average of the three principal stiffnesses, $\bar{\rho} = \frac{1}{3} \sum_{n=1}^{3} \rho_n$, on $\ln L$ is shown in figure 1 for various values of $H$. In this figure the solid lines are the low temperature $T = 0.2$ RG predictions and the points are the Monte Carlo results. The data points agree very well with the predictions of the NL$\sigma$ model at this low temperature. The stiffnesses decrease proportional to $\ln L$ and the results indicate that there is no stiffness at large length scales. Hence it would appear that the finite layer systems behave in the same way as the single layer system with no indication of a finite temperature phase transition in the stiffnesses. However, as the the number of layers increases the slopes of the lines in figure 1 decrease indicating that the stiffnesses should approach a finite value at large length scales as the system becomes fully three dimensional.

The excellent agreement of the Monte Carlo results and the RG predictions above indicate that topological excitations are not important in this system at low $T$.

However, at higher temperatures they may play an important role. These topological degrees of freedom are not included in the RG analysis. In order to study the vortex degrees of freedom directly, we have also calculated the response of the system to the presence of a single virtual vortex. We calculate this vorticity response for a fixed number of layers $H$ and for various linear sizes $L$. In figure 2 the temperature dependence of the vorticity data for $H = 2$ is shown. The curves for different sizes $L$ all cross at a common temperature point near $T = 0.51$. This behavior suggests that there is a free energy cost to creating isolated vortices in the system below this temperature but that they should spontaneously appear above it. At any value of $T$ we can study the size dependence of the vorticity using equation 2 to extract the coefficient of the $\ln L$ term which we call a vorticity modulus.

The vorticity moduli have been determined for systems

![FIG. 1: Average spin stiffness plotted as a function of $\ln L$ for different layer thicknesses $H$ at $T = 0.2$. The solid lines are the low temperature RG predictions.](image1)

![FIG. 2: Vorticity data for $H = 2$ and different linear sizes $L = 18, 30, 42, 60, 72$ as function of temperature.](image2)
having a different number of layers $H$. In each case, the vorticity moduli abruptly drop to zero at the same temperature where the vorticity curves cross. Figure 3 shows the average vorticity moduli $v = 4 \sum_{n=1}^{3} v_n$ multiplied by the layer thickness $H$ as a function of temperature for several layer thicknesses. The solid line represents the ratio $Hv/T = 1/\pi$ which intersects the corresponding layer vorticity modulus at the temperature where the raw vorticity curves cross. This suggests that the average vorticity modulus exhibits a universal jump, $v(T) = 1/(\pi H)$, at the transition which decreases as the number of layers $H$ increases.

Figure 4 shows a plot of $T_c(H)$ as well as the temperature of the specific heat maximum versus the inverse number of layers. As $\frac{1}{H} \to 0$ the system becomes three dimensional with the critical temperature equal to $T_c(3d) = 0.958$. The specific heat maxima lie above the temperatures where the vorticity moduli drop to zero but the two temperatures merge together as $1/H \to 0$.

The data points can be fit very well by a slightly modified form of the usual finite scaling (FSS)

$$T_c(H) = T_c(3d) \left(1 - \frac{C_1}{(H + H_1)^{\nu}} \right)$$

where both $C_1$ and $H_1$ are constants. The correlation length exponent $\nu$ in the above expression is the value for the three dimensional case and equals $\nu = 0.59$. Attempted fits of the data in figure 4 (solid line) using this form with $H_1 = 0$ are only possible for large values of $H > 8$ and there are strong deviations for smaller values of $H$. The dotted line in figure 4 corresponds to the values $C_1 = 7.28$ and $H_1 = 3.06$. This modified form provides an excellent fit over the entire range of layer thicknesses.

The quantity $H + H_1$ behaves as an effective layer width which may be related to the boundary conditions at the upper and lower surfaces. Figure 5 shows the average vorticity modulus $v(z)$ for each individual layer for the case of $H = 14$. The dotted horizontal curve is the average over all layers. The deviations of $v(z)$ from the average are larger for thin films than for thicker films. For small values of $H$ the effect of surface layers is significant and in the vicinity of the critical point the thickness $H$ is not the only relevant length scale. It is being modified by the additional constant $H_1$ which is related to how quickly $v(z)$ changes near the surface due to the free boundary conditions.

Modifying finite scaling theory to include the effective width for small $H < 8$ predicts that the vorticity moduli $v$ should scale with respect to the layer thickness $H$ as follows

$$(H + H_1) v = f((H + H_1)^{1/\nu}[t]).$$
where $\nu = 0.59$ is the three dimensional correlation length exponent and $t$ is the reduced temperature $(T_{c}(3d) - T_{c}(H))/T_{c}(3d)$. Figure 6 shows a plot of $H_{\text{eff}}$ in terms of the variable $H_{\text{eff}}^{1/\nu}|t|$. The vorticity moduli curves for different thicknesses collapse onto a universal curve.

The results above are similar to those found in studies of $^4$He superfluid films. In these systems the order parameter is a complex number which has the same symmetry as the ferromagnetic $XY$ model. The superfluid transition in $d = 2$ can be described in terms of the Kosterlitz-Thouless transition where vortices destroy the ordered phase. Ambegaokar et al. argued that the KT theory can be extended to films of finite thickness and that the transition should continue to have the 2d character provided the thickness is not too large. Schulthk and Manousakis have studied the same problem numerically and found that the results could indeed be described by the KT theory using finite scaling theory. However, a detailed fit for a small number of layers required the introduction of an effective width for the films. Our results for the frustrated Heisenberg model are quite similar but there are some important differences. In the $XY$ model, the transition is accompanied by a jump in the stiffness with a power law decay of the correlations below this temperature. This behavior persists for films of arbitrary thickness until the $3d$ bulk limit is reached where the transition becomes the usual $\lambda$ transition. In our case, the $d = 2$ behavior observed for a single layer also persists as the number of layers increases. The stiffness is zero at all finite $T$ indicating that the spin correlations decay exponentially at all temperatures. However, the vorticity modulus exhibits a universal jump at a finite temperature indicating that a topological phase transition occurs involving vortices. The size of the jump varies as $1/H$ and hence approaches zero in the limit of $d = 3$. In addition, the stiffness also approaches a nonzero value at temperatures below the critical temperature in this same limit. This indicates that the $2d$ behavior approaches the $3d$ behavior in a continuous way and that topological excitations play an important role between the two limits. The actual role that they play in determining the nature of the transition in $3d$ is still not clear. It is possible that the Heisenberg model has a weak first order transition as predicted by the NPRG field theories and that the critical exponents are only effective exponents. However, the evidence for first order behavior is much clearer for the $XY$ model and the differences between Heisenberg and $XY$ behavior may in fact be due to the different types of topological defects.

Acknowledgments

This work was supported by the Natural Sciences and Research Council of Canada and the HPC facility at the University of Manitoba and HPCVL at Queen’s University.

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