27. ON THE NATURE OF THE PHASE TRANSITION IN HELIMAGNETS

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Abstract: The nature of the phase transition in body-centered tetragonal helimagnets with both XY and Heisenberg spins is studied by extensive Monte Carlo simulations. In the XY case, evidence of a first order transition associated with the loss of helical ordering is found. The dependence on the turn angle Q is shown. In the Heisenberg case, only one second order transition is found. Critical exponents α and ν are calculated using finite size scaling.

I. INTRODUCTION

There has been a growing interest in the phase transition in helimagnets both experimentally and theoretically. However, its nature is still a subject of controversy. Experimentally, measurements of specific heat [1-3] in rare-earth metals Tb, Dy and Ho at the helical-paramagnetic transition were interpreted as evidence of a second order (SO) transition. However, other experiments suggested a weakly first order (FO) transition in Tb [4], Dy [5] and Ho [6]. On the other hand, data on Eu [7] and Cr [8] show a FO transition. Theoretically, Barak and Walker [9] found by a Renormalization Group (RG) calculation evidence of a FO transition in contradiction with early RG calculation [10]. Garel and Pfeuty [11] found that the transition depends on the number of spin components and on the turn angle Q between spins of adjacent layers . Dzyaloshinskii [12] showed that with exchange interaction alone only FO transition is possible in helimagnets. A recent analysis of the nature of helical transition in many-component spins in an arbitrary dimension d has also been done [13], but the case of d=3 with XY and Heisenberg spins was not conclusive, On the other hand, recent Monte Carlo (MC) simulations [14] for stacked antiferromagnetic triangular layers (AFT) were interpreted as evidence of a SO transition for both XY and Heisenberg spins.

II. MODEL AND TECHNIQUE

In this paper, we consider a body-centered tetragonal (bct) lattice . The Hamiltonian is written as

$$H = -J \sum_{ij} S_i . S_j \; - J' \sum_{ik} S_i . S_k \qquad (1)$$

where S_i is either an XY or a Heisenberg spin of unit length at the site i. J and J' are exchange integrals between spins in the (111) directions and along the c-axis, respectively. Here, both J and J' are taken to be negative to represent helical antiferromagnetic materials . Let η be the ratio J'/J (>0). Physical quantities will be measured in units of |J|.

The turn angle between spins belonging to two adjacent (basal) planes perpendicular to the c-axis is given by

$$\cos(Q) = -1/\eta \qquad (2)$$

The helcal structure is therefore stable for $\eta > 1$ ($90° <$ Q <

180°). For the XY case, the appropriate order parameter for helical ordering is defined as follows:

$$K = (1/4N) \langle \Sigma_{ij} \sin(\Theta_j-\Theta_i) \rangle / |\sin(\Theta_j^o-\Theta_i^o)| \qquad (3)$$

where the sum runs over all neighboring spin pairs in the four upward (111) directions, $(\Theta_j-\Theta_i)$ and $(\Theta_j^o-\Theta_i^o)(=Q)$ are the turn angles measured in the oriented XY plane at finite and zero temperature, respectively.The angular brackets in Eq. (3) denote thermal average at the temperature T and N is the total number of spins.

In this work, only following values of Q commensurate with the lattice periodicity are considered: Q = 105, 120, 150 and 165 degrees which correspond to η = 3.863703, 2, $2/\sqrt{3}$ and 1.035276, respectively. The magnetic cell is 12, 3, 6 and 12 times the original lattice cell along the c-axis for these respective values.

The lattice size is N= 2xLxLxL$_z$ with LxL being the number of lattice sites in each basal plane and L_z that along the c-axis. The sizes used are L=20 and L_z up to 24 for the XY case and L=L_z up to 21 for the Heisenberg case. Periodic boundary conditions have been used . Care must be taken to choose L_z commensurate with Q.

The MC method used is a multi-flipping procedure proposed by Creutz [15] . It has been tested and the convergence to equilibrium is much better than the single flipping procedure for a given CPU time. In our runs 15000 to 20000 MC flipping trials per spin were discarded to equilibrate the system before averaging physical quantities over the next 15000 to 20000 steps at each temperature. These runs are several times longer than previous MC runs [14]. Both heating and cooling were used with very small interval of successive temperatures. Many independent runs were been done to check the results shown below.

III. RESULTS

In this Letter, only essential results are shown. Details and analysis will be given in a full paper [16].

For XY spins, it is found that the finite temperature properties depend strongly on Q, namely η. For very strong η, i.e. Q is closer to 90°, a FO transition from helical to paramagnetic phase is found. Fig. 1 shows the internal energy per spin U versus T for Q=105° and Q=120°: U undergoes an appreciable discontinuity at the transition temperature T_c. The discontinuity is also found in K and in the basal plane magnetization A defined as

$$A = (1/N) \Sigma_p \langle M_p \rangle$$

where $\langle M_p \rangle$ is the thermal average of the magnetization of the basal plane p. Fig. 2 shows K and A versus T for Q=105° . The susceptibility χ associated with the fluctuations of A has also been calculated. It approaches T_c from below as a delta function but shows fluctuations above the transition. These fluctuations are small in magnitude when Q is close to 90° and becomes appreciable when Q increases [16]. A close inspection of all MC data reveals that these are due to the disordering of the basal

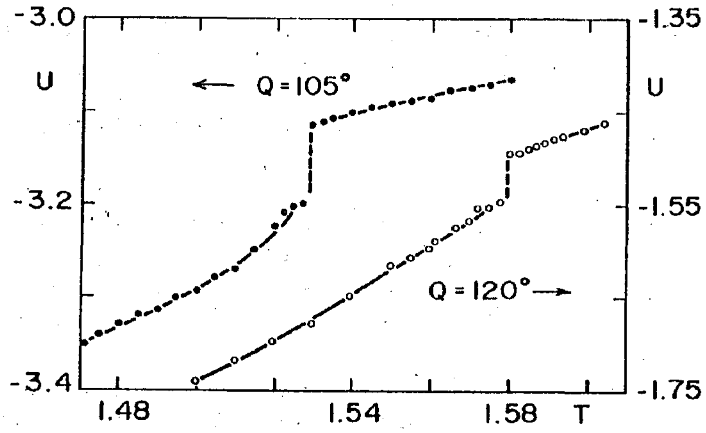
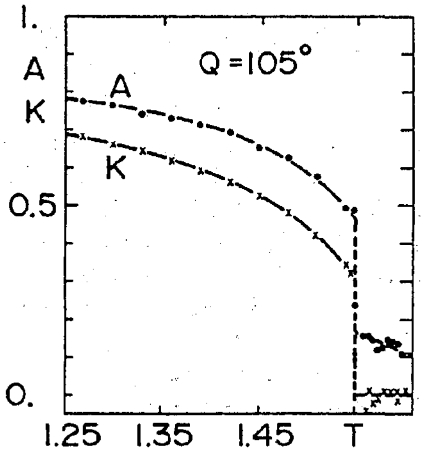


Fig.1 :XY case. Internal energy per spin U versus T for Q=105° (solid circles, left scale, L=20, L_z=24) and Q=120° (open circles, right scale, L=20, L_z=18). Lines are guides to the eye.



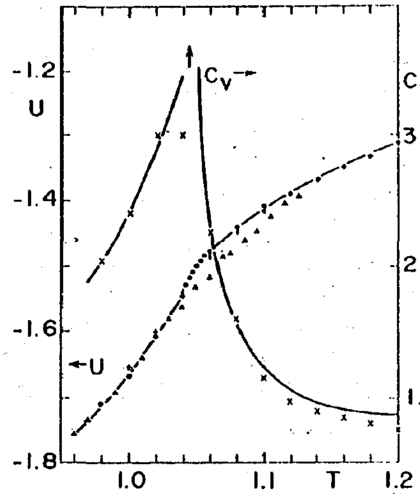


Fig.2 :XY case. Basal plane magnetization A and chiral order parameter K versus T (solid circles and crosses,respectively) for Q=105° , lattice sizes are given in Fig.1.

Fig.3 :Heisenberg case. U versus T for Q=120° with $L=L_z=9$ (triangles), 15(crosses) and 21 (circles). Data for sizes 6, 12 and 18 are not shown to preserve the clarity. Curve is drawn for size 21. C_v calculated by fluctuations (x) and by differentiating U with respect to T (solid line) is shown for size 21. The peak of C_v at 4.9 is shown by the vertical arrow.

planes which seems to take place at the same or just above but so close to T_c that it is impossible to distinguish within our MC resolution for these values of Q. The fluctuations are also seen in the specific heat above T_c [16]. They give rise to a separate SO transition when Q becomes larger as is shown later. We tried to calculate the hysteresis width Δ by slow heating and cooling but Δ is indistinguishable within our MC resolution. Experimentally, direct measurement of Δ was not possible, only by an extrapolation that Zochowski et al [5] found for Dy Δ=0.2

K which is to be compared to T_c=180 K.

The finite size effects at this FO transition is shown elsewhere [16].

When Q increases a SO transition associated with the loss of basal intra-plane ordering is observed at T_F. The results for Q=165° show that the helical transition is a FO one occurring at T_c=1.830 and the basal intra-plane ordering is broken at T_F=1.925 with a SO character [16]. The case Q=150° shows similar features to the case Q=165° except that the interval between T_c and T_F is smaller [16]. The ordering between T_c and T_F can be described as follows: each basal plane is still ferromagnetic due to interaction between spins of adjacent layers but it fluctuates between two opposite chiralities. The existence of one or two transitions depending on Q may be due to the change of behavior of the classical energy which is maximum at Q=135° [16]. The change from one FO transition at Q=105° and 120° to two transitions at Q=150° and 165° suggests that Q=135° is a multicritical point. Further studies are needed to check this.

In the Heisenberg case, only one SO transition is found for all the values of Q studied here. The physical reason for the disappearance of the FO character may be due to the fact that the system can go from one chiral state to the other by gradual distortion with the help of the third "escape" dimension of the Heisenberg spins.

Fig.3 shows U versus T for Q=120° together with the specific heat per spin C_v for L=L_z=21. Using the finite size scaling , one obtains the critical exponent ν = 0.570 ± 0.02 and α = 0.32 ± 0.03 [16].

The cases where Q=105, 150 and 165 degrees [16] show a SO character very similar to the case Q=120° presented above.

Let us first compare our results with existing theoretical calculations. The FO transition found here for the XY case is in agreement with Refs.[9] and [12] and the commensurate case of Ref.[11].However, theoretical calculations did not predict a SO transition occurring at a higher temperature. The temperature range for the intermediate phase depends on the value of Q, namely η. When Q is closer to 90°, these two transitions coincide, making only one FO transition within our MC resolution.

Our results for the XY case do not agree with the SO transition obtained in Ref.14 for AFT. The reason has been discussed in Ref. 16.

For the Heisenberg case, we obtained the critical exponents which are in agreement with those obtained in Ref.14. It is noted that for the Heisenberg case, our result does not agree with RG calculations by the order of the transition [9,11,12].

The FO transition observed in Eu [7] and Cr [8] is in agreement with our result for the XY case, although these elements have band magnetism (rather than localized spins) and complex sinusoidal spin structures. Tb, Dy and Ho have hcp structure and RKKY interaction different from the model studied here, so only general aspects will be compared . The FO transition found here for the XY case is in agreement with some experiments on these elements [4-6], but in disagreement with the SO transition observed by Jayasuriya et al [1-3]. This contradiction can be resolved if the spins in these materials are neither completely XY nor purely Heisenberg spins because the former would give a FO helical-paramagnetic transition while the latter would yield a SO one. Rather, they are Heisenberg spins with strong easy plane anisotropy: this will give a weak FO transition or a nearly SO one depending on the strength of anisotropy. That may be the reason why there was no universality in the measured values of α and β and no agreement about the nature of the transition.

NOTE ADDED IN PROOF:

The FO character found in the XY case has raised some suspicion [17]. This is based on the argument that Q may be temperature-dependent so that periodic boundary condition applied along the c axis may induce the FO character. I note that while for quantum Heisenberg spins it has been found that Q depends slightly on T by taking into account magnon-magnon interactions [18](Q is temperature-independent if free spin-wave theory is used), it is not evident that it is so for classical spins studied here. Large-scale simulations with L_z up to a few hundreds are now in progress to check the FO nature. If this is due to the periodic boundary condition, the FO character will be weakened with increasing size.

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