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MONTE CARLO SIMULATION OF THE TWO-DIMENSIONAL CLASSICAL HEISENBERG MODEL WITH EASY-PLANE ANISOTROPY

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Results of a classical Monte Carlo study of certain two-dimensional, nearest-neighbor Heisenberg model magnets are presented. An example with 1% easy-plane anisotropy is described in detail. Here there is evidence for a Kosterlitz-Thouless-like topological phase transition at temperature $T=T_{KT}$ with $T_{KT} \simeq 2/3T_{KT}$(planar limit). A specific heat anomaly occures at $T_s > T_{KT}$. In-plane spin-component correlations decay exponentially for $T > T_{KT}$ and as a power law for $T < T_{KT}$, whereas out-of-plane correlations appear exponentially for all T but, interesting, with anomalies around both T_{KT} and $\sim T_s$.

1. Introduction

We have undertaken [1,2] a numerical (Monte Carlo) study of a range of two-dimensional (2-d) ferromagnetic and anti-ferromagnetic classical Heisenberg models. A variety of spin anisotropies are being examined: isotropic [1], uniaxial, XY with (e.g. crystal field) symmetry-breaking fields in the (xy) easy-plane. The primary motivation of this work is not to study phase transitions (e.g. critical exponents) in great detail. Other techniques such as RG Monte Carlo [3] can then be much more appropriate. Rather we wish to understand the types of, and competitions between, strongly nonlinear spin excitations (e.g. vortices, domains). The variety and thermodynamic consequences of such excitations are much greater in 2-d than 1-d, but the range (in temperature, for example) of essentially 2-d fluctuations can still be much greater than in 3-d. This program of study is now especially appropriate in view of the renewed theoretical appreciation of strongly nonlinear phenomena, coupled with a new experimental emphasis on studying 2-d materials as well as re-assessments of existing examples---e.g. planar magnets (K_2CuF_4, Rb_2CrCL_4, ---); magnetic lipid layers prepared by the Langmuir-Blodgett technique [4]; magnetic epitaxial systems (e.g. O_2 on a non-magnetic substrate); layered compounds with magnetic intercalates (e.g. graphite with transition metal Chlorides [5] or transition metal Dichalcogenides [6]). The greater body of our work is still in progress and will be described elsewhere. Here we focus on one specific case [2] motivated by the recent interest [7] in K_2CuF_4, a planar ferromagnetic with only approximately 1% easy-plane spin anisotropy. The apparent absence of symmetry-breaking in the easy-plane [7] and the weak magnetic coupling between planes ($J_{/\!/}/J_{\perp} \sim 10^4$) leads one to anticipate a reasonable regime of predominantly 2-d fluctuations around the ultimately 3-d transition temperature. Furthermore, the general phenomena ascribed to bound and unbound vortex configurations (referred to below as Kosterlitz-Thouless (KT) theory [8]) can be anticipated.

(to be contrasted with the isotropic limit[1,3].) Our results are consistent with the growing experimental data on K_2CuF_4 as described by Hirakawa[7] even though S=1/2 and quantum effects are not yet included. In addition we are able to study out-of-plane fluctuations and find indications of unexpected structure. In formation on the out-of-plane behavior should be increasing probed, for example as a means of studying vortex dynamics[8].

2. Results

The Hamiltonian we studied is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z) \, , \qquad (1)$$

where $J > 0$ is the nearest-neighbor exchange constant, $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$ and $0 \leq \lambda < 1$. We have studied several values of λ but will consider here $\lambda = 0.99$, having in mind K_2CuF_4 [7]. Recall that the planar limit ($\lambda = 0$) is now well-understood by KT theory[9]. MC simulations[10,11] have supported this picture and suggest $T_{KT}(\lambda = 0) \simeq 0.9$ J with an additional specific heat "maximum" at $T_s \simeq (1.0-1.05)J$. Universality suggests that we should have the same critical exponents for spin fluctuations in the easy-plane(xy) for all λ in [1], with the same universal jump in η, etc. Of course scales (as for the spin-wave theory) depend on λ, but indeed <u>vortices</u> can occur for all $\lambda < 1$ with cores much as for $\lambda = 0$ (contrast the instantons in $\lambda = 1$ [1]). Free energy estimates then show that $T_{KT}(\lambda) \sim T_{KT}(0)/\ln(1-\lambda)^{-1/2}$ in agreement with RG treatments. Thus $T_{KT}(\lambda) \to 0$ very slowly as $\lambda \to 1$, the isotropic Heisenberg limit, and even for $\lambda = 0.99$ we expect a substantial transition temperature. In fact we find $T_{KT}(0.99) = (0.60-0.65)J$ which is in fair accord with the incipient 2-d KT transition temperature (mitigated by 3-d ordering) as interpreted [7] in K_2CuF_4. We have used a conventional MC algorithm[1,2] with typically 6×10^3 steps, random initial spin configurations, and periodic boundary conditions on 10x10, 20x20, 30x30 and 40x40 square lattices. Fig.1 shows specific heat (C_v) results. Note the near extensive behavior and the evidence for a specific heat maximum at $T_s(0.99) = (0.65-0.70)J \simeq 2/3 T_s(0)$ (above). This Shottky-like anomaly is less sharp than in the planar limit ($\lambda = 0$) since out-of-plane fluctuations are easier. As expected, the mean energy was also found to be extensive with no indication of a phase transition. To estimate the critical temperature T_{KT}(0.99) we have studied (i) the size-dependence of $\langle M^2 \rangle / N$ (N is the number of spins) and the susceptibility $\chi \equiv (k_B T N)^{-1} (\langle M^2 \rangle - \langle M \rangle^2)$ and (ii) power-law and exponential fits tovarious spin-spin correlation functions. The susceptibility should be extensive for $T > T_{KT}$ (above discussion), but N-dependent for $T \;\; T_{KT}$ with [10]

$$k_B T \chi = \langle M^2 \rangle / N \propto N^{1-1/2\,\eta(T)} , \qquad (2)$$

where we have assumed $\langle M \rangle = 0$. Results for the exponent $a(T) = 1-1/2\,\eta(T)$ deduced from [2] are shown in Fig.2. Fig.3 illustrates structure observed in $\langle M_z^2 \rangle$ (i.e. out-of-plane component) in the critical region. The structure is reminiscent of that in C_v but we have not yet been able to assign a maximum in the range $0.6 < T < 0.7$: our best estimate of $T_{KT}(0.99)$ is o.62-0.63 (below). We have made power-law and exponential fits to the spatial decay of spin-spin correlations $\langle \vec{S}_0 \vec{S}_n \rangle$, $\langle S_0^x S_n^x \rangle$ and $\langle S_0^z S_n^z \rangle$ [2]. As expected the in-plane critical fluctuations are consistent with power-law decay for $T < T_{KT}$ and exponential for $T > T_{KT}$, with $T_{KT}(0.99) = (0.62-0.63)J$. We have used the $T < T_{KT}$ data as an alternative way to estimate a(T) (see above) and the results are shown in Fig.2. Our finite system results tend to under-estimate $a(T < T_{KT})$ as in the planar limit[10]. The out-of-plane correlations contain interesting new information. Our fits imply an exponential decay of $\langle S_0^z S_n^z \rangle$ correlations for $T > T_{KT}$ and $< T_{KT}$. In addition we find evidence for two anomalies at T_{KT} and in the neighborhood of T_s: see, for example, the correlation lengths (extracted from best exponential fits for $\langle \vec{S}_0 \vec{S}_n \rangle$ and $\langle S_0^z S_n^z \rangle$) plotted as functions of T. This unusual behavior probably rejects intrinsic crossovers but we are cheking for artificial numerical biases. (in Fig.4).

In summary, our results indicate a KT type transition in the classical Heisenberg model with easy-plane anisotropy. The critical temperature is $T_{KT} \simeq 2/3$ the planar limit value even with only 1% anisotropy. In addition we find a broad specific heat anomaly at $T_s \simeq 1.1 T_{KT}$. Out-of-plane correlations decay exponentially for $T > T_{KT}$ and $T < T_{KT}$ and are sensitive to both T_{KT} and T_s. More details of our continuing studies of the easy-plane and other models will be published later.

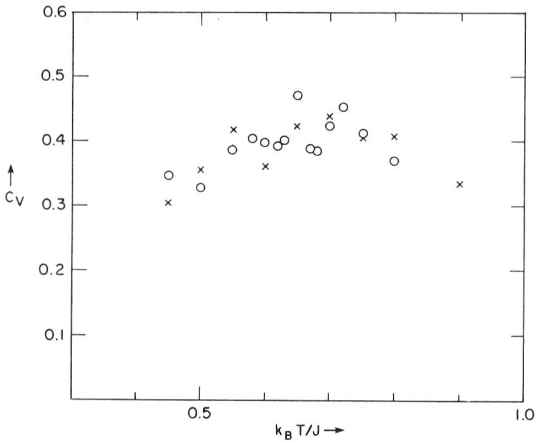

Fig.1

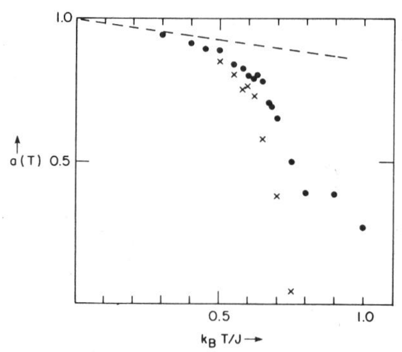

Fig.2

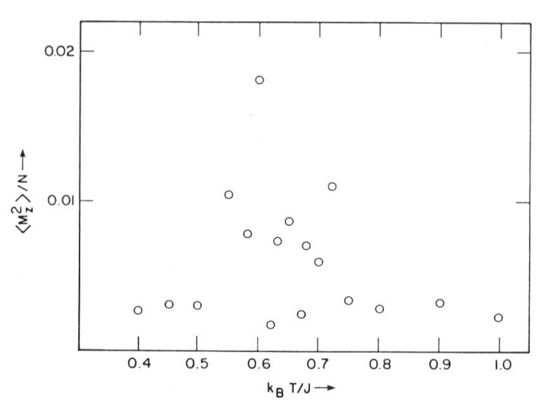

Fig.3

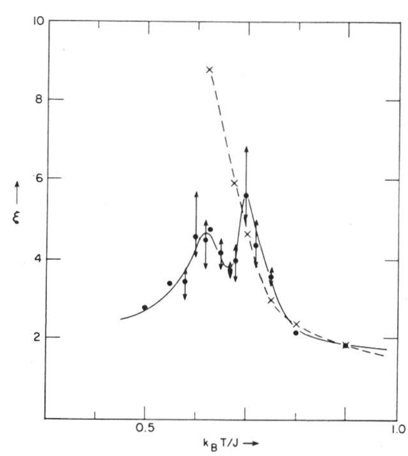

Fig.4

Fig.1 Specific heat C_V, computed as $(2/k_BT)^2(k_B/N)(\langle E^2\rangle - \langle E\rangle^2)$, 30x30 (×) and 40x40 (o) lattices.

Fig.2 Exponent a(T) (see text) computed from in-plane correlation functions (×) and susceptibility (●). The dashed line (---) is spin-wave theory.

Fig.3 Mean square out-of-plane magnetization $\langle M_z^2\rangle/N$ for 40x40 lattice. The corresponding susceptibility is described in the text.

Fig.4 Correlation lengths ξ (in lattice spacings) for $\langle \vec{S}_0 \vec{S}_n\rangle$ (×) and $\langle S_0^z S_n^z\rangle$ deduced from best exponential fits. The error indicate fitting uncertainties and are not estimates of intrinsic MC uncertainties. The solid and dashed lines are guides to the eye.

References

[1] C.Kawabata and A.R.Bishop: Solid State Commun.33(1980)453.
[2] C.Kawabata and A.R.Bishop: Solid State Commun.42(1982)595.
[3] S.H.Shenker and J.Tobochinik: Phys.Rev.B22(1980)4462.
[4] M.Pomerantz: in Phase Transitions in Surface Films,eds. J.Ruvalds(Plenum,NY,1980),p.317.
[5] M.Elahy,C.Nicolini,G.Dresselhaus andG.O.Zimmerman: Solid State Commun.41(1982)289.
[6] S.S.P.Parkin and R.H.Friend: Phil.Mag.41(1980)65 and 95.
[7] K.Hirakawa: Proceedings of international conference on magnetism and magnetic materials, Atlanta(U.S.A), November(1981).
[8] D.L.Huber: in ordering in two-dimensions,ed.S.K.Sinha (North-Holland,NY,1980),p.417.
[9] J.M.Kosterlitz and D.J.Thouless: Prog.Low.Tem.Phys. (ed.D.F.Brewer), Vol.VIIB(North-Holland, Amsterdam,1978).
[10] S.Miyashita,et.al: Prog.Theor.Phys.60(1978)1669.
[11] J.Tobochinik and G.V.Chester: Phys.Rev..B20(1979)3761.
J.E.Van Himbergen and S.Chakravarty: Phys.Rev.B23(1981)359.