ADDITIONAL EVIDENCE FOR A PHASE TRANSITION IN THE PLANE-ROTATOR AND CLASSICAL HEISENBERG MODELS FOR TWO-DIMENSIONAL LATTICES*

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High-temperature series expansions of the spin-spin correlation functions of the plane-rotator and classical Heisenberg models have been obtained to order $(J/kT)^{10}$ on the triangular lattice. An analysis of the moment series provides good evidence for a phase transition.

Recently considerable experimental and theoretical attention has been directed toward two-dimensional magnetic systems.[1-9] Experiments have shown that very long-range antiferromagnetic order, completely two-dimensional in character, exists in K_2NiF_4 from 97.1 to at least 200 °K.[2] It has also been rigorously proved that the two-dimensional isotropic Heisenberg model with finite-range exchange interactions cannot be ferromagnetic or antiferromagnetic.[6] Stanley and Kaplan[4] have suggested that a phase transition may still take place, even though the magnetization remains zero in the low-temperature phase.[7] Their evidence for a phase transition was mainly derived from the behavior of the high-temperature series expansion of the susceptibility of the Heisenberg ferromagnet on the plane triangular lattice. Eight terms were then known for the classical (infinite spin) Heisenberg model, and six terms for general spin values. Stanley later found similar behavior for the plane-rotator (or planar) model on two-dimensional lattices.[5] The classical Heisenberg and plane-rotator models are described by the Hamiltonian

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j, \tag{1}$$

where $\vec{S}_i$ is a D-dimensional classical spin of magnitude $D^{1/2}$, and the sum is taken over all nearest-neighbor sites i and j. For the classical Heisenberg model, $D=3$, while for the plane-rotator model, $D=2$. The plane-rotator model is of interest as it is expected to have the same critical behavior as the transition from a normal liquid to a superfluid.[10] We have found the high-temperature series expansion of the spin-spin correlation function $\Gamma(\vec{r},T)$ through order $(J/kT)^{10}$ for the Ising, plane-rotator, and classical Heisenberg models on the triangular lattice. The two additional terms thereby generated in the susceptibility series support the original conclusions of Stanley and Kaplan.[4,5] We have obtained what we believe is much stronger evidence for a phase transition by analyzing in addition the inverse moment series of $\Gamma(\vec{r},T)$. It is possible, of course, that the interpretation of the series analysis in terms of a phase transition is incorrect.[11] Even if this is the case, the series will still be of much value for fitting to experimental data.[3]

The method used in obtaining the series expansion is an extension of the procedure previously used on the three-dimensional Ising model.[12] That is, we used the Englert[13] linked-cluster expansion, but completely renormalized in the sense of De Dominicis.[14,15] The computer program which is being used at present is only efficient for the Ising model. For the plane-rotator and classical Heisenberg model, it becomes very wasteful of computer time because of the large number of needless repetitions of the lattice counts for the perturbation diagrams. This defect seems inherent in the method. The advantage of the method is that the human effort required for the programming is small. The best chance of obtaining more terms probably lies in modifying the vertex-renormalized form of the Englert expansion, previously used by Jasnow and Wortis.[16]

The spherical moments of the correlation function[17] are defined by

$$\mu_t=\sum_{\vec{r}}r^t\Gamma(\vec{r},T)=\sum_n m_n^{(t)}K^n, \tag{2}$$

where $K=J/kT$. The quantities $m_n^{(0)}$ are the coefficients of the usual dimensionless susceptibility series, while $m_n^{(2)}$ are the coefficients of the second-moment series. Table I contains susceptibility and second-moment coefficients for the Ising, plane-rotator, and classical Heisenberg models for the triangular lattice. In the three-dimensional versions of these models and in the two-dimensional Ising model, μ_t has a leading singularity at the critical point of the type

$$\mu_t\sim(1-K/K_c)^{-(\gamma+t\nu)},\ \text{as } K\to K_c, \tag{3}$$

where γ is the susceptibility index ($t=0$) and ν is the index describing the dependence of the corre-

Table I. Expansion coefficients of the zeroth and second correlation moments in powers of K on the triangular lattice.

	Ising		Plane Rotator		Heisenberg	
n	$m_n^{(0)}$	$m_n^{(2)}$	$m_n^{(0)}$	$m_n^{(2)}$	$m_n^{(0)}$	$m_n^{(2)}$
1	6	6	6	6	6	6
2	30	72	30	72	30	72
3	136	580	135	579	134.4	578.4
4	586	3 864	570	3 834	560.4	3 816
5	2 448.8	22 968.8	2 306	22 520	2 219.726	22 250.126
6	10 021.333	126 451.2	9 041.5	121 754	8 450.194	118 923.154
7	40 364.876	658 598.476	34 582.125	619 004.125	31 131.456	595 173.861
8	160 627.295	3 288 792.229	129 634.167	3 000 084.417	111 528.736	2 827 401.396
9	633 205.211	15 888 299.814	477 988.033	13 991 240.117	389 998.632	12 869 466.046
10	2 477 249.529	74 731 776.570	1 738 252.392	63 207 887.650	1 335 034.608	56 505 807.622

lation length on $(1-K/K_c)$.[17] If (3) still holds for two-dimensional systems with a continuous symmetry, i.e., the plane-rotator and Heisenberg models, then we should expect to find that the ratios of successive terms in the tth-moment series (which we shall denote by $\rho_{t,n}$) approach K_c^{-1} as $n\to\infty$. Successive ratios from $n=6$ to $n=10$ of $\rho_{0,n}$ for the Heisenberg model are 3.8069, 3.6841, 3.5825, 3.4968, and 3.4232. Extrapolation of these ratios against $1/n$ suggests that a finite limit, around 2.4, is eventually reached. This was the original evidence of Stanley and Kaplan[4] for a phase transition. One cannot help but wonder whether with more terms the value $K_c^{-1}=0$ might be obtained, especially in view of the rapid decrease in the values of the ratios.

Before discussing evidence against this hypothesis we remark that, in contrast to the case of the two-dimensional Ising model and the three-dimensional versions of the plane-rotator and classical Heisenberg models, the coefficients in the series expansion of $\Gamma(\vec{r}, T)$ for the plane-rotator and Heisenberg models are not all positive. Table II gives their values to the nearest-neighbor site. In general, the coefficients are all negative beyond the sixth or seventh nonvanishing term to a given site, at least to the order we know them. The series to the more distant sites, for which we have less than six nonvanishing terms, have positive coefficients and closely resemble those of the Ising model. The more distant sites make a large contribution to the second-moment series, and a smaller contribution to an inverse ($t<0$) moment series, due to the r^t weighting factor. Conclusions about the existence of a phase transition based on the behavior of $t\geq 0$ moment series are necessarily suspect, since they contain less of the information in the spin-spin correlation function which is distinctively non-Ising. The same cannot be said of the inverse-moment series, which stress the contributions from sites near the origin, and the series with negative coefficients. It is shown below that analysis of the inverse-moment series yields values for K_c compatible with those derived from the positive-moment series. We believe this constitutes strong evidence for a phase transition.

The ratios $\rho_{t,n}$ of the plane-rotator model for $t=-1.75$ are, from $n=6$ to 10, 2.8063, 2.8067,

Table II. Expansion coefficients of $\Gamma(\vec{r},T)$ at the nearest-neighbor site.

n	Ising	Plane rotator	Heisenberg
1	1	1	1
2	2	2	2
3	3.666 667	3.5	3.4
4	6.666 667	5	4
5	14.133 333	5.833 333	0.754 286
6	36.088 889	4.666 666	−14.08
7	98.879 365	−5.062 500	−61.523 429
8	277.206 349	−52.347 222	−200.875 102
9	798.159 436	−229.390 278	−577.065 588
10	2 360.482 821	−782.100 001	−1 462.243 658

2.7930, 2.7842, and 2.7860. Notice that the last term does not follow the usual trend of ever decreasing estimates for K_c^{-1}. This change in direction is more clearly seen on studying the linear extrapolants $l_{t,n}$ defined by

$$l_{t,n} = n\rho_{t,n} - (n-1)\rho_{t,n-1}. \tag{4}$$

Figure 1 shows a plot of $l_{t,n}$ vs $1/n(n-1)$ for a variety of values of t. (It is logical to extrapolate in this fashion if $\rho_{t,n}$ can be developed in a power series in $1/n$.) Moment series with both positive and negative t values extrapolate to roughly the same value of K_c^{-1}, around 3.15 ± 0.10. For values of t close to -2, the turn-up starts to disappear. Extrapolation with the aid of a Neville table,[16] which automatically allows for curvature in the plot, suggests that with only slightly longer series the same value for K_c^{-1} would still be obtained. A hint of similar behavior can be found in the series for the Heisenberg model. That only a hint can be found is because the series for the Heisenberg model are more like those of the spherical model than are the series for the plane-rotator model.[5] The spherical model does not have a phase transition in two dimensions, a fact reflected in the behavior of the susceptibility series.[9] The turn-up also suggests that every coefficient in the susceptibility series of the plane-rotator model could be positive, in contrast to the case of the spherical model whose susceptibility coefficients oscillate in sign irregularly beyond the 13th term.[9]

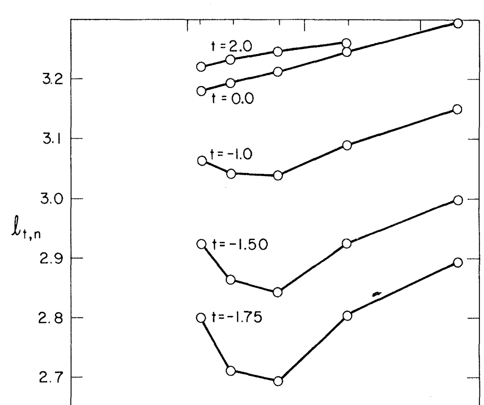

FIG. 1. Linear extrapolants of various moment series of the plane-rotator model. The turn-up seen in the last two terms suggests that T_c is bounded away from zero.

In conclusion, the evidence from moment series for a phase transition in the plane-rotator model is as strong in two dimensions as it is in three. Assuming that a transition does take place, and that (3) is valid, we find that for the plane-rotator model, $\gamma = 3.0 \pm 0.5$ and $\nu = 2.0^{+1.0}_{-0.5}$. We do not believe the series are yet long enough to estimate the indices of the Heisenberg model.

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