# POSSIBILITY OF A PHASE TRANSITION FOR THE TWO-DIMENSIONAL HEISENBERG MODEL

H. E. Stanley
Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts, and
Lincoln Laboratory,* Massachusetts Institute of Technology, Lexington, Massachusetts

and

T. A. Kaplan
Lincoln Laboratory,* Massachusetts Institute of Technology, Lexington, Massachusetts
(Received 16 August 1966)

We point out that the existence of a phase transition—as indicated by extrapolation from high-temperature expansions—is as well-founded for two-dimensional lattices with nearest-neighbor ferromagnetic Heisenberg interactions as for three-dimensional lattices, and that the "well-known result" that there exists no phase transition in two dimensions is not a valid conclusion from the standard spin-wave argument.

It has commonly been supposed that the two-dimensional Heisenberg model with nearest-neighbor ferromagnetic interactions will not undergo a phase transition. In this Letter, we present evidence based on high-temperature extrapolation methods which indicates the presence of a phase transition just as convincingly for two-dimensional Heisenberg models (with $S>\frac{1}{2}$) as for three-dimensional cases.[1] Furthermore, we show that the "well-known result" that the two-dimensional critical temperature $T_c^{(2)}$ vanishes is not a valid conclusion from the standard spin-wave argument.[2] We also observe that the high-temperature methods suggest a simple power-law divergence of the zero-field susceptibility at $T_c$, $\chi\sim(T-T_c)^{-\gamma}$, with $\gamma\cong 8/3$ in two dimensions, and that $T_c^{(2)}$ depends on spin and lattice in a fashion analogous to the dependence found for three-dimensional cubic lattices.

The basic idea behind the extrapolation method of determining $T_c$ is that one seeks the radius of convergence of the power series representation of the susceptibility, $\chi\propto\sum_l a_l(J/kT)^l$, given only the first several $a_l$. An extrapolation procedure frequently used involves plotting the ratios of successive terms $a_l$ vs $1/l$. Curve (a) of Fig. 1 is a plot for a three-dimensional example, the simple cubic lattice ($z=6$) with $S=\frac{3}{2}$. The observation that this plot appears to approach a straight line for large $l$ motivates the extrapolation to $l=\infty$ (dashed line) and the identification of the intercept with the reciprocal of the radius of convergence, i.e., with $T_c$. (Since $a_1\propto T_M$, the ordering temperature predicted by the Weiss molecular field approximation, we have plotted $a_l/a_1a_{l-1}$ in order that the intercept be $T_c/T_M$.) Moreover, if $\chi$ is to diverge as $T\to T_c^+$ with a power law, $\chi\sim(T-T_c)^{-\gamma}$, then for large $l$, $a_l/a_1a_{l-1}\cong(T_c/T_M)[1+(\gamma-1)/l]$. Indeed, the slope of the plot in Fig. 1(a) corresponds to $\gamma\cong1.38$, consistent with the results of a Padé-approximant analysis.[3]

We have calculated the $a_l$, $l\leq 6$, for three different two-dimensional lattices. Curve (a) of Fig. 2 shows $a_l/a_1a_{l-1}$ vs $1/l$ for the plane triangular lattice ($z=6$) with $S=\frac{3}{2}$. We notice at once that the ratios of successive terms seem to approach a straight line for large $l$ in a manner which is actually more regular than that of our three-dimensional example; hence, the extrapolation $l\to\infty$ can be made with an even greater degree of credibility than in the three-dimensional case. For the example of Fig. 2, we estimate $T_c/T_M=0.435\pm0.01$; the slope of the straight line corresponds to $\gamma=2.75\pm0.05$.[4]

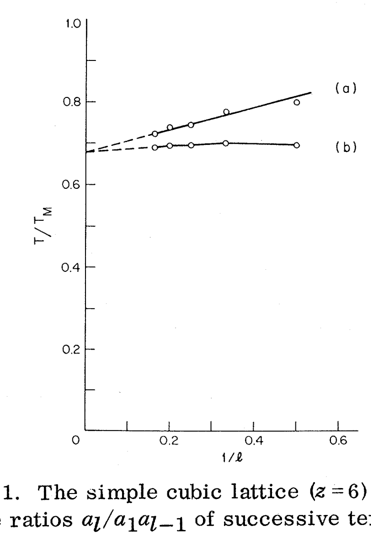


FIG. 1. The simple cubic lattice ($z=6$) with $S=\frac{3}{2}$. (a) The ratios $a_l/a_1a_{l-1}$ of successive terms in the susceptibility series are known only for $l\leq 6$. Extrapolating to $l\to\infty$, one estimates $T_c/T_M\cong 0.68$. (b) The function $t_l(\gamma'=\frac{4}{3})$.

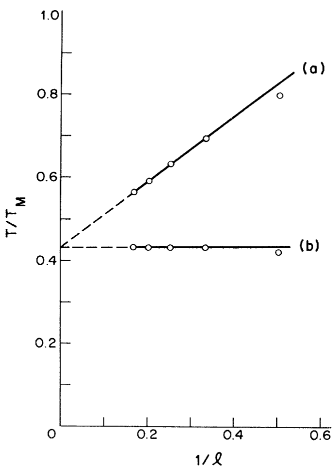


FIG. 2. The plane triangular lattice ($z=6$) with $S=\frac{3}{2}$. (a) The ratios $a_l/a_1a_{l-1}$ approach $T_c/T_M \cong 0.435$. (b) The function $t_l(\gamma'=2.75)$. As in Fig. 1, the coefficients $a_l$ were obtained from the general expressions of Rushbrooke and Wood,[1] valid for any spin and lattice.

Curves (b) in Figs. 1 and 2 represent an application of the Domb-Sykes[5] criterion for determining $\gamma$. If $\chi$ does diverge with a power law, then for $\gamma'=\gamma$ the plot of $t_l(\gamma') \equiv (a_l/a_1a_{l-1}) \times[1+(\gamma'-1)/l]^{-1}$ vs $1/l$ should approach $T_c/T_M$ with zero slope. We used many "trial values" $\gamma'$ and again found $\gamma = 2.75 \pm 0.05$ for the two-dimensional example of Fig. 2.

We performed the above analyses for $S=\frac{1}{2}$, 1, $\frac{3}{2}$, 2, $\frac{5}{2}$, 3, 5, 10, $\infty$ for the plane triangular ($z=6$), the plane square ($z=4$), and the honeycomb ($z=3$) lattices with nearest-neighbor ferromagnetic interactions. We found, for all but the $S=\frac{1}{2}$ case, a well-defined $T_c^{(2)} \sim T_M/2$. (For $S=\frac{1}{2}$ the $a_l$ do not behave sufficiently regularly to estimate $T_c^{(2)}$.) As in three dimensions, the estimated $T_c^{(2)}$ vary regularly with $z$ and $S$ (for $S>\frac{1}{2}$), fitting, to within a few percent, the simple formula[6]

$$kT_c^{(2)}/J \cong \tfrac{1}{5}(z-1)[2S(S+1)-1]. \tag{1}$$

Equation (1) is completely analogous to the formula given by Rushbrooke and Wood[1] for three-dimensional cubic lattices. Also, just as for the three-dimensional case,[7] there is a slow but nevertheless clear variation of $\gamma$ with $S$. For $S>\frac{1}{2}$ and $z>3$, we find $\gamma^{(2)}(S) \cong \frac{5}{2}+2/(3S^2)$, as compared with $\gamma^{(3)}(S) \cong \frac{4}{3}+1/(20S)$.[7] In summary, the coefficients $a_l$ behave regularly with $l$ for a given $S>\frac{1}{2}$ and lattice—at least as regularly for two- as for three-dimensional lattices; also, the extrapolated values of $T_c$ and $\gamma$ vary smoothly with $S$ and $z$—just as smoothly for two- as for three-dimensional lattices. We conclude that the existence of a phase transition, as indicated by extrapolation from high-temperature expansions, is as well founded in two as it is in three dimensions.

Let us now review the standard spin-wave argument[2] against the existence of a phase transition for the two-dimensional Heisenberg ferromagnet. It consists of a "proof" that the spontaneous magnetization is zero for all positive temperatures. The essential physical assumption is that at sufficiently small $T$ the spins are nearly $\hat{z}S$, the $x$ and $y$ components being small. This assumption leads to various mathematical approximations which in turn lead to the well-known result[2] that the change in average spin per particle $\delta S \equiv S - \langle S_z\rangle_T$, although small for three-dimensional lattices (at small $T$), is infinite in one and two dimensions (at any $T>0$). Thus there appears to be a contradiction, implying that the original assumption of the smallness of $\delta S$ is incorrect. The very common "physical" interpretation of this result is that the true value of $\langle S_z\rangle_T$ is really zero in one and two dimensions (rather than the literal value, $-\infty$). That is, there is no spontaneous magnetization at positive $T$; this is generally taken to imply that there exists no phase transition in one or two dimensions. We wish to point out that this standard spin-wave argument is not a valid proof that there exists no phase transition, there being two errors: (i) The nonexistence of a spontaneous magnetization at positive $T$ does not imply that no phase transition exists (the spin correlations may be of a qualitatively much longer range below some nonzero critical temperature $T_c^{(2)}$ than above—this possibility is discussed in detail in the next paragraph). (ii) The spin-wave argument as it stands does not imply the vanishing of the spontaneous magnetization because the mathematical approximations made have not been rigorously shown to be consequences of the physical assumption that $\delta S$ is small.[8]

What, then, happens for $T<T_c^{(2)}$? Here we can only discuss various possibilities.[9] Our result that $\chi(T)$ (which is proportional to $\sum_R \langle \vec{S}_0\cdot\vec{S}_R\rangle_T$) diverges as $T$ approaches $T_c^{(2)}$ definitely means that at $T_c^{(2)}$ the spin-correlation function $\Gamma(R) \equiv \langle S_0\cdot S_R\rangle_T$ becomes very long range. For example, if we assume $\Gamma(R) \propto R^{-\lambda}$ for large $R$, our result means that $\lambda \leq 2$

at $T = T_c^{(2)}$. Intuitively, we expect that[10] $\chi(T)$ will not decrease with decreasing $T$ (although we could not prove it). If so, then $\chi = \infty$ for all $T < T_c^{(2)}$, so that $\lambda(T) \leq 2$ for $T \leq T_c^{(2)}$. This clearly includes the case of "ordinary" ferromagnetism, for which $\lambda = 0$ $(T < T_c)$. It also includes the possibility that $\lambda > 0$, in which case the saturation magnetization would be zero and the curve of $M$ vs $H$ would have an infinite derivative at $H = 0$ without having a finite discontinuity.[11]

In summary, then, the evidence from high-temperature expansions indicates the presence of a phase transition just as clearly in two dimensions as in three and, although there exist various[12] nonrigorous "proofs" that $M = 0$ for all positive $T$, there are no arguments (so far as we know) which preclude the possibility of a phase transition. The nature of the suggested low-temperature phase is being investigated.

---

*Operated with support from the U. S. Air Force.

[1]In their monumental work on high-temperature expansions G. S. Rushbrooke and P. J. Wood, Mol. Phys. 1, 257 (1958), observed that "there is no evidence that the two-dimensional lattices do not have Curie temperatures." However, they mitigated the strength of their observation by adding that "firm conclusions are more difficult to draw from the coefficients" in the two-dimensional cases they considered than in the three-dimensional cases. They gave no reason for this mitigation; in the present Letter, we show that it is unwarranted.

[2]See, for example, F. Bloch, Z. Physik 61, 206 (1930); J. Van Kranendonk and J. H. Van Vleck, Rev. Mod. Phys. 30, 1 (1958); and F. Keffer, "Spin Waves" (to be published).

[3]J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) 275, 257 (1963), Table III.

[4]The errors indicated are, as usual, the results of a subjective judgment, and are not meant to be precise. No matter how one judges "where the coefficients are going" as $l$ increases, it is clear from curves (a) in Figs. 1 and 2 that for consistency, the errors on $T_c^{(2)}$ should be no greater than those on $T_c^{(3)}$.

[5]C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962).

[6]Comparison of (1) with Rushbrooke and Wood's corresponding mnemonic formula for the three-dimensional cubic lattices $kT_c^{(3)}/J = (5/96)(z-1)[11S(S+1)-1]$ suggests that the classical or "infinite-spin" approximation is better in three than in two dimensions.

[7]H. E. Stanley and T. A. Kaplan, to be published.

[8]More precisely, the mathematical approximations consist basically of replacing the operator $S_{jz}$ by the operator $|[S(S+1)-S_{jx}^2-S_{jy}^2]^{1/2}|$, which in turn is replaced by its formal expansion in powers of $S_{jx}^2+S_{jy}^2$ up to the first power of $S_{jx}^2+S_{jy}^2$ in the energy and the zeroth power in the relation $[S_{jx}, S_{jy}] = iS_{jz}$. The "justification" is essentially the statement that as $T \to 0$, the approach of $\delta S$ to zero implies that the matrix elements of $S_{jx}^2+S_{jy}^2$ between the states which are statistically important approach zero. That much more is needed in the way of justification can be seen strikingly for the case $S = \frac{1}{2}$: then $S_{jx}^2 = S_{jy}^2 = \frac{1}{4}$, which, being constant for all states (including even the ground state), obviously is no smaller for states important at low temperature than for any other states.

[9]One should not forget that the high-$T$ extrapolation method is not rigorous. Thus the indicated transition could be spurious, a possibility which we, however, feel is unlikely.

[10]Our

$$\chi \equiv \lim_{N\to\infty} \lim_{H\to 0} \frac{\partial M}{\partial H}$$

is useful for conceptual reasons. It differs from another $\chi$, commonly used, in which the order of the limits is reversed. Our $\chi$ is given for all $T$ by $(g^2\mu_B^2/3kT)\sum_R \Gamma(R)$.

[11]We have used the relationship $\Gamma(R) \to S_T^2$ as $R \to \infty$, where $\vec{S}_T$ is the average spin per site. [See L. Van Hove, Phys. Rev. 95, 1374 (1954), Eq. (27).]

[12]Another "proof" that $M = 0$ for $T > 0$ is given in G. H. Wannier, Elements of Solid State Theory (Cambridge University Press, London, England, 1959), pp. 111-113.