On the Possible Phase Transition for Two-Dimensional Heisenberg Models

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Recently the authors presented evidence suggesting the presence of a phase transition for two-dimensional Heisenberg models with nearest-neighbor ferromagnetic interactions and $S>\frac{1}{2}$. Here we further analyze the first six coefficients of the high-temperature series for the zero-field susceptibility, and incorporate the results of recent calculations beyond sixth order into the arguments for a phase transition. It is found that the higher-order coefficients support the previous suggestion concerning the existence of a phase transition for $S>\frac{1}{2}$, and are consistent with a zero critical temperature for the particular case $S=\frac{1}{2}$. Finally, two preliminary calculations on the nature of the low-temperature phase are described. The first of these, due to Dyson, is an intuitive generalization of spin wave theory. The other is an approximate calculation for the rectangular net within the classical Heisenberg model: Considering this net to consist of linear chains, the intrachain interactions are treated exactly, while the interchain interactions are treated via a molecular field approximation. Both of these calculations support the original suggestion of a phase transition for two-dimensional Heisenberg models.

It has commonly been supposed that the two-dimensional Heisenberg model with nearest-neighbor ferromagnetic interactions will not undergo a phase transition. Recently, the opposite has been suggested[1] for spin quantum number $S>\frac{1}{2}$. This suggestion was based on the behavior of the first six terms in the high-temperature expansion of the zero-field susceptibility χ, and on a discussion pointing out that the previous arguments against the existence of such a phase transition are not substantial. Here we further analyze these coefficients, and incorporate the results of recent calculations beyond sixth order into the arguments for a phase transition for $S>\frac{1}{2}$. Also, some preliminary calculations on the nature of the low-temperature phase are described.

We recently pointed out that for some two-dimensional lattices the ratios a_l/a_{l-1} of successive terms in the high-temperature series expansion of the zero-field susceptibility $\chi\sim\sum_l a_l(J/kT)^l$, when plotted against $1/l$, seem to approach a straight line for large l in a manner which is as regular as for three-dimensional cases.[1] Hence the extrapolation to $l=\infty$ and the identification of the intercept with a critical temperature T_c can be made as reliably in two dimensions as in three. In Fig. 1 we plot T_c vs $S(S+1)$ for the simple cubic and plane triangular lattices, and note that T_c varies with S as smoothly in two as in three dimensions. We also find a smooth variation of the two-dimensional critical temperature $T_c^{(2)}$ with coordination number z for the triangular ($z=6$), square ($z=4$), and honeycomb ($z=3$) lattices. This variation with $S(>\frac{1}{2})$ and lattice is conveniently summarized (to within a few percent) by the formula

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

A notable exception to the regular variation with l of the a_l occurs for the case $S=\frac{1}{2}$, where the a_l do not behave sufficiently regularly to estimate $T_c^{(2)}$ reliably. However, the value of S for which the plot of $T_c^{(2)}$ vs $S(S+1)$ in Fig. 1 passes through zero is very nearly $\frac{1}{2}$, suggesting that perhaps there is no phase transition for $S=\frac{1}{2}$. The high-temperature series has recently been extended for $S=\frac{1}{2}$ by methods practicable only for $S=\frac{1}{2}$, 1.[2,3] Both Refs. 2 and 3 give numerical values of the new coefficients only for selected three-dimensional lattices, but Eq. (27) of Ref. 2 expresses one additional term for the close-packed lattices, and three additional terms for the loose-packed lattices, in terms of basic lattice properties. From these, a_7 for the triangular lattice and a_7-a_9 for the square and honeycomb lattices have been calculated.[4] Unfortunately, the additional terms do not reduce the irregularity for the case of $S=\frac{1}{2}$, and hence reliable extrapolations of the a_l for $S=\frac{1}{2}$ would still seem to be impossible.

There has been recent interest in taking advantage of the tremendous simplifications which occur in the *classical* Heisenberg model.[5] This model is of particular interest in connection with the basic question considered in the present paper, since it presents the same "di-

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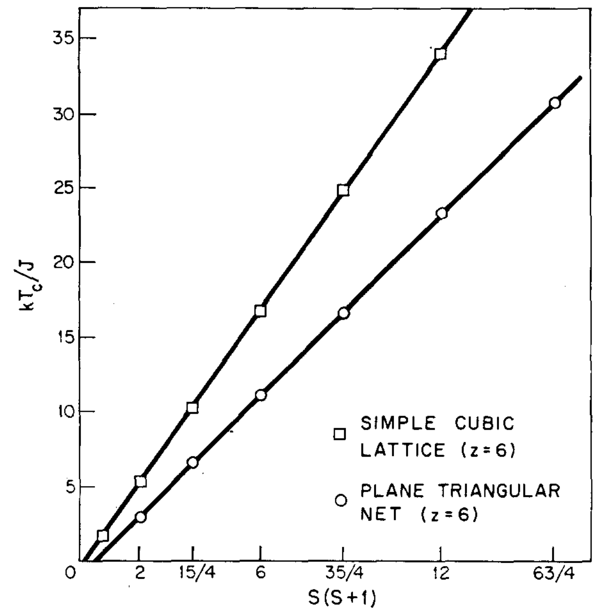

FIG. 1. The variation of the extrapolated estimates of the critical temperature with spin quantum number S for the (three-dimensional) simple cubic and for the (two-dimensional) plane triangular lattices.

lemma" as that which occurs quantum mechanically: Arguments plausible at low temperatures lead to a magnetization which is infinite in one and in two dimensions, finite in three dimensions,[6] whereas the high-temperature expansion coefficients strongly suggest a phase transition at a nonzero temperature in two as well as in three dimensions (but not in one). Therefore calculations have been made[7] on two-dimensional lattices: the new coefficients obtained are a_7 for the triangular lattice and a_7-a_9 for the square and honeycomb lattices. *The additional terms in these classical cases support the conclusion, already drawn*[1] *from the first six terms, that there probably is a phase transition.*

High-temperature expansion methods have been used to predict not only the radius of convergence J/kT_c of the power series representation of χ but also the *form*[8,9] of the divergence of χ as $T\rightarrow T_c^+$. If one assumes the divergence to be of the form $\chi\sim(T-T_c)^{-\gamma}$, one finds[10] that for the three-dimensional cubic lattices $\gamma^{(3)}(S)\cong 1.33+0.05/S$. We have discovered an analogous variation with $S(>\frac{1}{2})$ for the square and triangular lattices.[1] The results of using both the Domb–Sykes[8] criterion and a related criterion $\{$that for large l, $a_l/a_{l-1}\simeq(kT_c/J)[1+(\gamma-1)/l]\}$ are completely summarized—to within a few percent—by $\gamma^{(2)}(S)\cong 2.+5\,0.67/S^2$.

What, then, happens for $T<T_c^{(2)}$? Here we can only discuss various possibilities. Our result that $\chi(T)$ (which is proportional to $\sum_R\langle S_0\cdot S_R\rangle_T$) diverges as T approaches $T_c^{(2)}$ 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 $\chi(T)$ will not decrease with decreasing T.[11] 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 $\lambda>0(T<T_c)$, in which case *the saturation magnetization would be zero* and the curve M vs H would have an infinite derivative at $H=0$ without having a finite discontinuity.

We discussed with Dyson the evidence from the high-temperature expansions that $T_c^{(2)}\neq 0$. He has since argued,[12] on the basis of an intuitive generalization of spin-wave theory, that $M=0$ for $T>0$, and that at low temperature, $\Gamma(R)\sim R^{-\lambda}$ for large R, with λ linear in T.

We also considered, for the classical Heisenberg model, an approximate calculation for the rectangular net. Considering this net to consist of linear chains, the intrachain interactions (J) are treated exactly, while the interchain interactions (J') are treated via a molecular field approximation. This calculation gives a spontaneous magnetization in two (and three) dimensions, but not in one. The critical temperature obtained in this calculation is nonzero for any nonzero values of J and J', approaching zero (the correct limit) continuously as $J'/J\rightarrow 0$; moreover, the value for the two-dimensional square net is less than 50% larger than the result (1) based upon high-temperature expansions.

Note added in proof: Recently Mermin and Wagner[13] proved that the spontaneous magnetization is zero for two-dimensional lattices with short-range interactions. Consequently, the phase transition suggested by the high-temperature expansion would have to be of the zero-magnetization type discussed above. We note that the Mermin–Wagner result shows that the molecular-field-type approximation described above overestimates the stability of long-range order, as has been known to happen in molecular-field calculations involving small clusters.

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