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Numerical Evidence for the Existence of a Phase Transition in a Two-Dimensional Exchange-Interaction Model

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High-temperature–low-field susceptibility series for the exchange-interaction model of ferromagnetism are analyzed by means of a reexpansion technique to obtain the ordering temperature. In particular, for all two-sublattice decomposible structures (e.g., linear chain, plain square, simple cubic, body-centered cubic) the formula $k_B T_C/J = (12/5)(z - 5/2)(4S+3)^{-1}$ reproduces our numerical results.

I. INTRODUCTION

Bogoliubov-type arguments have been used to rule out the possibility of a "phase transition" in two-dimensional lattices for a wide class of isotropic interaction Hamiltonians.[1] On the other hand, Stanley and Kaplan[2] have shown, using high-temperature series, that the numerical evidence for a phase transition in the two-dimensional (2-d) Heisenberg model (HSB) is just as convincing as for the three-dimensional (3-d) case. The major criticism of their result seems to have been that the available series are too short to yield reliable evidence for 2-d systems. A theoretical resolution to this dilemma has been proposed by Stanley and Kaplan[3] who point out that one must be clear in distinguish-

ing between the existence of a spontaneous magnetization in which case the zero-field correlation function is finite in range $M^2 \propto \lim_{r\to\infty} \langle S_0 S_r\rangle \neq 0$ and the weaker condition for a phase transition where the correlation function is sufficiently long-ranged that the zero-field isothermal susceptibility diverges $\chi_T \propto \sum_r \langle S_0 S_r\rangle = \infty$. The purpose of the present paper is to present what we feel is convincing numerical evidence for the existence of a phase transition, in the latter sense, for a 2-d exchange-interaction ferromagnet (EX). To do this we have made an extensive reexpansion analysis of the known[4] high-temperature susceptibility series for the exchange-interaction model (eight terms for general crystal lattices) and the existence of a finite T_C is exhibited.

II. THEORY

We consider a ferromagnetic system containing N particles of spin S with isotropic nearest-neighbor exchange interaction. The exchange-interaction Hamiltonian is given by

$$\mathcal{H} = -J \sum_{\langle ij\rangle} P_{ij} - g\mu_B H \sum_{i=1}^{n} S_{z_i} \ . \tag{1}$$

Here P_{ij} is the Schrödinger exchange operator and is a polynomial of degree $2S$ in $\vec{S}_i \cdot \vec{S}_j$:

$$P_{ij} = \sum_{n=0}^{2S} A_n(S)\,(\vec{S}_i \cdot \vec{S}_j)^n, \quad i \neq j \ . \tag{2}$$

The coefficients A_n are determined from the property that P_{ij} exchanges, or permutes, the spin coordinates of two atoms labeled i and j:

$$P_{ij}\,O(i,j) = O(j,i)\,P_{ij} \ , \tag{3}$$

where $O(i,j)$ is any operator which contains the spin operators of atoms i and j. Typical forms for the operator P_{ij} are

$$\begin{aligned} P_{ij} &= \tfrac{1}{2} + 2(\vec{S}_i \cdot \vec{S}_j); \quad S = \tfrac{1}{2} \\ &= -1 + (\vec{S}_i \cdot \vec{S}_j) + (\vec{S}_i \cdot \vec{S}_j)^2; \quad S = 1 \\ &= -\tfrac{67}{32} - \tfrac{9}{8}(\vec{S}_i \cdot \vec{S}_j) + \tfrac{11}{16}(\vec{S}_i \cdot \vec{S}_j)^2 + \tfrac{2}{9}(\vec{S}_i \cdot \vec{S}_j)^3; \\ &\qquad S = \tfrac{3}{2} \ , \quad \text{etc.} \end{aligned} \tag{4}$$

Due to the permutation property of the Schrödinger exchange operator P_{ij}, high-temperature series can be extended further with less effort for this model than for the Heisenberg model. For the case $S = \frac{1}{2}$ the two models are identical. Chen and Joseph[4] obtained eight terms in the low-field–high-temperature susceptibility serves for arbitrary spin and general crystal lattices. The high-temperature–low-field susceptibility series can be written in the form

$$\chi \propto \sum_n a_n K^n \ , \tag{5}$$

where $K = J/k_B T$. If one assumes that near the critical temperature χ diverges as $(K_C - K)^{-\gamma}$, one then has for large n

$$a_n/a_{n-1} \sim (1/K_C)\,[1 + (\gamma - 1)n] \ . \tag{6}$$

Consequently, one makes plots of a_n/a_{n-1} vs $1/n$ and interprets the intercept $1/n = 0$ as $1/K_C$. Frequently, however, the series are too erratic to obtain reliable results. A more sophisticated method of analysis is hence called for.

The technique we have used is the method of conformal transformations[5] as used by Lee and Stanley[6] with certain modifications and extensions. Lee and Stanley have shown that if one introduces the transformed variable

$$K^* = K/(1 + tK) \ , \tag{7}$$

in terms of which we may write

$$\chi \propto \sum_n b_n (K^*)^n \ , \tag{8}$$

that by adjusting the parameter t, plots of b_n/b_{n-1} vs $1/n$ can be made to behave quite regularly. From such plots one then obtains $1/K_C^*$ and hence $1/K_C$ by using

$$1/K_C = 1/K_C^* - t \ . \tag{9}$$

Our method differs from that of Lee and Stanley[6] in two respects. First, we do not require a unique value of t to be used for all lattices and all spins. We sought, by computer techniques, the optimum value of t for each situation. Secondly, we have introduced the concept of a validity criterion for the reexpansion—"the validity fraction V." V is defined as the ratio of the number of points[7] on a b_n/b_{n-1}-vs-$1/n$ plot which fall on a straight line (l) to the total number of (data) points available (n), e.g., $V \equiv l/n$. It is clear that V can range from $V = 2/n$, representing the worst possible fit, to $V = 1$, where every point falls on the same straight line. As a practical matter, we found that results for which $V \geq (1/n)\,(1 + \frac{1}{2}n) = \frac{1}{2} + 1/n$ implied that a high level of confidence had been achieved. Results for which $V = \frac{1}{2}$ were also considered reliable but anything with $V < \frac{1}{2}$ was considered suspect. Figure 1 illustrates a typical t-parameter family and shows how we obtained our "best" extrapolated critical intercept. The numbers in parentheses are a reflection of the validity criterion just discussed.

Table I summarizes the results of our numerical analysis for $k_B T_C^{\mathrm{EX}}/J$ for a wide variety of 1-, 2-, and 3-d lattices for spin values from $\frac{1}{2}$ to 6. The numbers in parentheses refer to the validity fraction.

III. DISCUSSION

In order to see if there was any systematics in our results, various plots of T_C vs S and z (near-

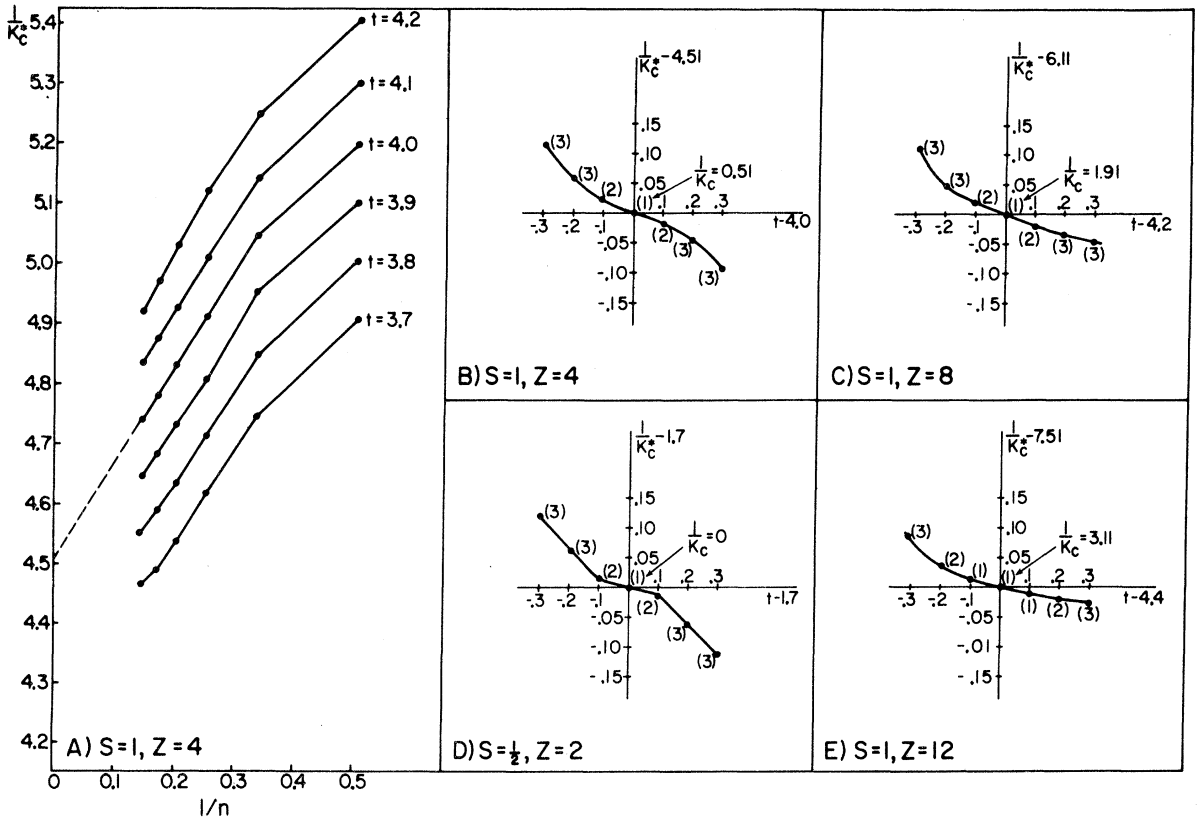

FIG. 1. (A) $1/K_C^*$ vs $1/n$ for various t for $S=1$, plane square; (B) $1/K_C^*-4.51$ vs $t-4.0$ for $S=1$, plane square; (C) $1/K_C^*-6.11$ vs $t-4.2$ for $S=1$, bcc; (D) $1/K_C^*-1.7$ vs $t-1.7$ for $S=\frac{1}{2}$, linear chain; (E) $1/K_C^*-7.51$ vs $t-4.4$ for $S=1$, fcc. In $B-E$, the numbers next to the points indicate the validity fraction V (see text for discussion): (1) $V=\frac{5}{8}$; (2) $V=\frac{1}{2}$; (3) $V=\frac{3}{8}$.

est-neighbor number)were made. In Fig. 2 we show the variation of $k_BT_C^{EX}/J$ with $(4S+3)^{-1}$ for the various lattices considered. To within our precision the curves are all straight lines for $S>\frac{1}{2}$. These critical temperatures can be summarized in the simple formula

$$k_BT_C^{EX}(S, L)/J=A(L)(4S+3)^{-1}+B(L)\,; \qquad (10)$$

here L denotes the lattice dependence. The result of a least-squares determination of the parameters A and B is given in Table II. A study of the dependence of A and B on L showed that for those

TABLE I. k_BT_C/J for the exchange-interaction model for various spin values and lattices. The numbers in parentheses indicate the validity fraction V (see text for discussion): (1) $V\geq\frac{5}{8}$; (2) $V=\frac{1}{2}$; (3) $V<\frac{1}{2}$.

S \ L	Linear	Honeycomb	Diamond	Plane square	Plane triangle	sc	bcc	fcc
$\frac{1}{2}$	0(1)	0.32(2)	0.83(2)	0.62(2)	0.87(2)	1.69(1)	2.53(1)	4.01(1)
1	−0.175(2)	0.18(2)	0.50(2)	0.51(1)	0.78(2)	1.20(1)	1.90(1)	3.11(1)
$\frac{3}{2}$	−0.14(2)	0.10(2)	0.36(2)	0.41(1)	0.67(2)	0.93(1)	1.47(1)	2.63(1)
2	−0.12(2)	0.05(3)	0.28(2)	0.33(1)	0.60(2)	0.76(1)	1.20(1)	2.34(1)
$\frac{5}{2}$	−0.10(2)	0.03(3)	0.22(2)	0.28(1)	0.56(2)	0.64(1)	1.02(1)	2.12(1)
3	−0.09(2)	0.01(3)	0.18(2)	0.24(1)	0.53(2)	0.55(1)	0.88(1)	1.96(1)
$\frac{7}{2}$	−0.075(2)	0(3)	0.14(3)	0.21(2)	0.50(3)	0.49(2)	0.77(1)	1.83(1)
4	−0.070(3)	−0.01(3)	0.11(3)	0.19(2)	0.48(3)	0.43(2)	0.69(2)	1.75(1)
$\frac{9}{2}$	−0.055(3)	−0.03(3)	0.09(3)	0.17(2)	0.46(3)	0.39(2)	0.62(2)	1.67(1)
5	−0.05(3)	−0.04(3)	0.08(3)	0.16(2)	0.44(3)	0.36(2)	0.57(2)	1.61(1)
$\frac{11}{2}$	−0.045(3)	−0.045(3)	0.07(3)	0.15(2)	0.43(3)	0.33(2)	0.52(2)	1.55(1)
6	−0.04(3)	−0.05(3)	0.06(3)	0.14(2)	0.42(3)	0.31(2)	0.49(2)	1.50(1)

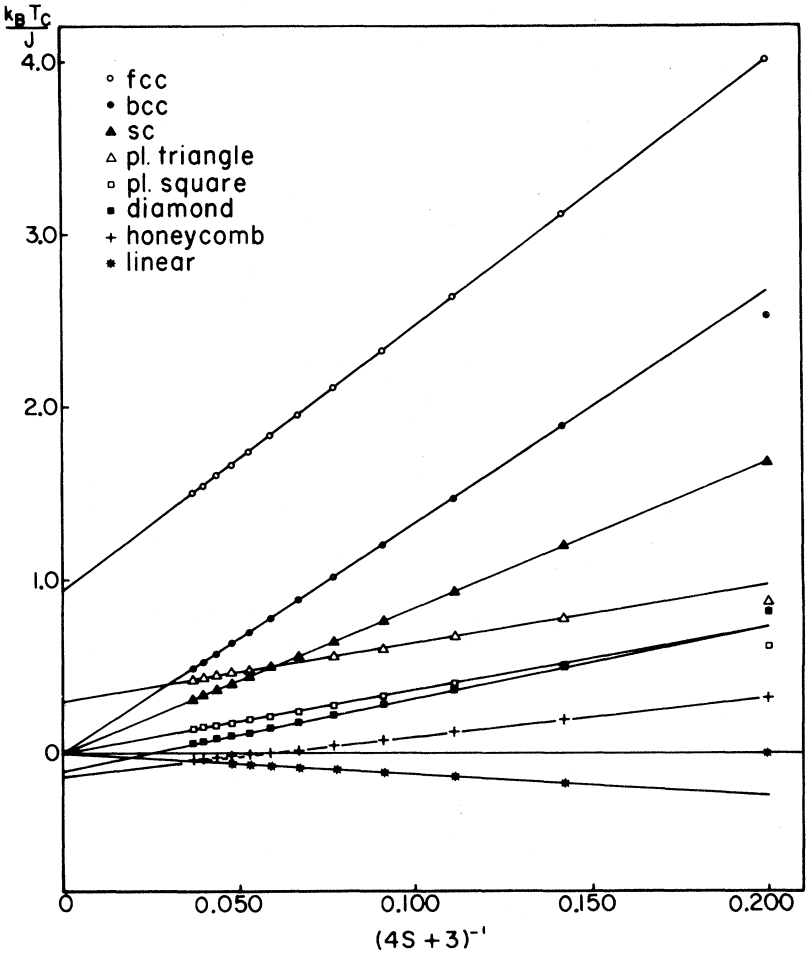

FIG. 2. $k_B T/J$ vs $(4S+3)^{-1}$ for exchange-interaction Hamiltonian for various lattices.

lattices which are simply decomposable into two sublattices, e.g., linear chain ($z=2$), plane square ($z=4$), simple cubic ($z=6$), and body-centered cubic ($z=8$), to within our precision, A and B are simply given by

$$A(z)=\tfrac{12}{5}(z-\tfrac{5}{2}),\quad B(z)=0. \tag{11}$$

T_C's for which $V\geq\frac{1}{2}$ have an associated error[7] of about ± 0.01, while for cases where $V<\frac{1}{2}$ the error[7] was considerably greater, in the range ± 0.05. This point is worth bearing in mind when one considers the extremely small values of T_C frequently found. In general the error increases with increasing S.

TABLE II. Coefficients $A(L)$ and $B(L)$ appearing in Eq. (10), for various lattices. z is the nearest-neighbor number.

Lattice (z)	$A(L)$	$B(L)$
Linear (2)	−1.22	0
Honeycomb (3)	2.23	−0.13
Plane Square (4)	3.58	0.01
Plane Triangle (6)	3.29	0.31
Diamond (4)	4.21	−0.10
sc (6)	8.42	0.01
bcc (8)	13.23	0.01
fcc (12)	14.88	0.98

We feel that considerable validity can be ascribed to the results for the three cubic lattices and for the 2-d plane-square lattice. For the 2-d honeycomb and triangular lattices, our confidence in the results is not as great, but for the lower spin values we feel the results are still to be trusted. A similar statement holds true for the 3-d diamond lattice. Consequently, the negative values of T_C which are obtained (or implied) for large spin values for the diamond and honeycomb lattices are felt to be spurious. Such solutions are clearly unacceptable on physical grounds.

For similar reasons, the negative T_C values found for the 1-d linear-chain lattice for $S>\frac{1}{2}$ are clearly spurious. The reason why we have included these negative values is to point out that in fact they agree quite closely with the values given by Eqs. (10) and (11), which connects lattices of dif-

ferent dimensionality. We believe this case amply illustrates the treachery inherent in the blind acceptance of numerical results based on finite series.

For $S=\frac{1}{2}$ (the Heisenberg case) there seems to be no simple systematic behavior to the calculated T_C. In general, these points do not fall too far from what Eqs. (10) and (11) would imply, but they are definitely outside the uncertainty limits that are ascribed to these points.

Suzuki[8] has shown that in a "strict" sense (the existence of a spontaneous magnetization) there are no phase transitions in ideal isotropic ferromagnets such as the Heisenberg and exchange models in two dimensions. He does not, however, rule out the possibility of other kinds of "weaker" phase transitions, such as might be associated with the divergence of the susceptibility. Furthermore, based upon the greater degeneracy of the exchange-models ground state—its higher symmetry and consequent lower point of broken symmetry—he has shown that any order parameter for the exchange model must be less than or equal to that of the Heisenberg model. If for example we consider the critical point associated with the divergence of the susceptibility T_C then

$$T_C^{\mathrm{EX}} \leq T_C^{\mathrm{HSB}} . \tag{12}$$

The present work based upon an eight-term series, coupled with new reexpansion techniques, gives what we feel is strong evidence for a phase transition (in the weaker sense) for the exchange model in two dimensions. Based upon the previously mentioned symmetry arguments, we believe that these results supplement and strengthen the direct evidence presented by Stanley and Kaplan[2] for such transitions in 2-d Heisenberg ferromagnets.

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Proof of a Conjecture by Luttinger and Tisza

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A conjecture of Luttinger and Tisza on the ordering of classical spins on a lattice is proven for a class of Bravais lattices with arbitrary spin-spin interactions, provided the interaction obeys a simple symmetry, and is restricted to nearest neighbors only. The proof holds for lattices in which all bonds lie along edges of stacked similar parallelepipeds.

The purpose of this paper is to discuss a conjecture of Luttinger and Tisza[1] about the ordering of classical spins in a configuration which minimizes the energy of a lattice of spins. Luttinger and Tisza (LT) have considered, in particular, the case of a simple cubic lattice with spins interacting via dipole-dipole forces and conjectured that the minimum-energy configuration is invariant under any translation by twice the lattice spacing. In this particular case, Onsager[2] had hinted earlier that there is a proof for the lowest-energy configuration, which indeed satisfies the LT conjecture. More recently there has been some interest on interactions via quadrupole-quadrupole forces,[3] which are relevant to ordering in molecular crystals, and it was conjectured that the minimum-en-