Odd-spin-cluster interactions

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We consider interactions of Ising spins three at a time, five at a time, etc., as distinguished from the conventional interactions (two at a time). To illustrate, we calculate the exact thermodynamics of three-spin-cluster interactions in one dimension with and without a magnetic field. We find regular structures except at a certain value of the coupling constant ratio ($J_1/J_3=-3$) where the ground state becomes chaotic. The $T\rightarrow 0$ limit of the magnetization agrees with the exact ground-state calculation.

This paper is intended to call attention to spin interactions in which products of odd numbers of spin operators are involved. In magnetic Hamiltonians, the perturbation due to an external magnetic field at the nth site involves the most trivial such cluster, containing a single spin. We write $J_1C_n^1$, where J_1 is the coupling constant (the strength of the external magnetic field), and C_n^1 is the one-spin cluster located at the nth site, i.e., S_n. In this paper we shall take the spins to be of the Ising type, i.e., each S_n equal to ± 1.

In a linear chain the simplest nontrivial odd-spin cluster takes the form of the product of three spins, $S_nS_{n+1}S_{n+2}$, which we shall denote C_{n+1}^3. Assigning a coupling constant J_3 to this interaction, we can construct a Hamiltonian

$$H=J_3\sum_n C_n^3+J_1\sum_n C_n^1 \tag{1}$$

and use it to calculate a partition function, from which one can calculate correlation functions and other thermodynamic properties at finite temperature T. This we shall do in the next section, finding results which differ from those for the usual Ising model based on binary clusters $C_n^2=S_nS_{n+1}$.

Clusters possess certain interesting properties which do not appear to have been noted heretofore. For example, take C_n^3. There are four configurations yielding $+1$ for this quantity: $+++$, $+--$, $-+-$, $--+$, and four configurations yielding -1: $---$, $-++$, $+-+$, $++-$. Supposing we restrict the cluster to one of the eigenvalues, for example, $+1$; there is one configuration of magnetization $M=3$, and three with $M=-1$, making the average zero. This result holds for any cluster size of two or more spins. Further, we conjecture that fixing the eigenvalue of any size cluster allows *any* smaller *odd*-spin cluster embedded within to average to zero.

The properties noted above are those of isolated clusters. Once we sum on clusters in a given lattice, the situation becomes more complex. For example, C_n^3 and C_{n+1}^3 have two spins (S_n and S_{n+1}) in common, and when both clusters are present as in the Hamiltonian (1), spin correlations must occur. This will be examined below.

In two dimensions, say on a square lattice, it is possible to have two distinct binary bonds (vertical, horizontal), six distinct ternary bonds (four right-angled, one horizontal, and one vertical), a number of quaternary bonds (although only one simple one—the square), and a "natural" five-spin cluster: the star illustrated in Fig. 1. Similarly, in the

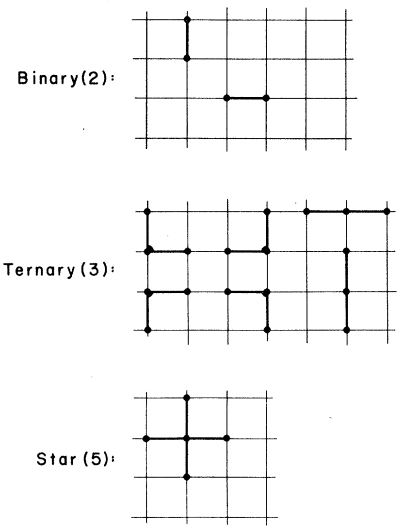

FIG. 1. A cluster interaction is the product of the spins connected by a heavy line. The binary clusters are the usual in an Ising model, the ternary and star clusters are the new-type clusters discussed in this paper.

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simple-cubic three-dimensional lattice, the seven-spin star cluster is the "natural" odd-spin cluster reflecting the point-group symmetry.

This paper concerns the mathematics and statistical mechanics of such generalized Ising systems. Possible applications are touched upon in the concluding section.

ONE DIMENSION

We start with $J_1=0$ in Eq. (1). The partition function is

$$Z=(2\cosh\beta J_3)^N \tag{2}$$

and the correlation functions are easily calculated,

$$M=\langle S_n\rangle=0,\quad \langle S_nS_{n+p}\rangle=0 \quad \text{for } p\neq 3\ (m=0,1,2,\ldots),$$
$$\langle S_nS_{n+3m}\rangle=\tanh^{2m}\beta J_3\ ,$$
and
$$\langle C^3_{n+1}\rangle=\langle S_nS_{n+1}S_{n+2}\rangle=-\tanh\beta J_3\ . \tag{3}$$

Interestingly, the two-spin correlations are independent of the sign of J_3 whereas the three-spin cluster correlation appropriately does depend on it.

We turn next to the general case $J_3,J_1\neq 0$. Evaluation of the partition function by the transfer-matrix method[1] yields a quartic equation:

$$z^4-[2\cosh\beta(J_1+J_3)]z^3+[2\cosh\beta(J_1+J_3)-2\cosh\beta(3J_3-J_1)]z+2[\cosh 4\beta J_3-1]=0\ . \tag{4}$$

The partition function Z equals z^N, where z is the largest root of (4). Thus the free energy *per* spin f is

$$f=-k_BT\ln z\ . \tag{5}$$

Various thermodynamic functions such as internal energy U, heat capacity C, magnetization M, and susceptibility χ, are all known derivatives of f, hence of z. They can be obtained by implicit differentiation of (4). For example,

$$U=-Nz^{-1}\partial z/\partial\beta\ ,$$

where

$$\frac{\partial z}{\partial\beta}=\{[(J_1+J_3)\sinh\beta(J_1+J_3)]z^3+[(3J_3-J_1)\sinh\beta(3J_3-J_1)-(J_1+J_3)\sinh\beta(J_1+J_3)]z-[4J_3\sinh 4\beta J_3]\}$$
$$\times\{2z^3-[3\cosh\beta(J_1+J_3)]z^2+[\cosh\beta(J_1+J_3)-\cosh\beta(3J_3-J_1)]\}^{-1} \tag{6}$$

with z the largest root of (4). In the calculation of heat capacity or specific heat, a second derivative is required; it is obtained by differentiating (6) further. For the magnetization, $\partial z/\partial J_1$ is required and for the magnetic susceptibility χ, a second derivative. They are all obtained similarly, but the expressions are too cumbersome to reproduce. Anyhow, all the desired thermodynamic functions are calculable directly by this method, without need for numerical differentiation—thus permitting us to obtain high precision without undue numerical computation.

It is not required to carry out the calculations for all J_1 and J_3, as the transformation $S_n\rightarrow -S_n$ (all n) is tantamount to a change in sign of both J_1 and J_3. We thus limit the phase space to be investigated to the region $J_1\leq 0$, fix the unit of energy by setting $J_1^2+J_3^2=1$, and express k_BT in these units. The magnetization, susceptibility, and specific heat computed for various representative ratios J_1/J_3 are given in Figs. 2–6. We note M always has the sign of $-J_1$ regardless of the sign of J_3; $M=0$ at all T for $J_1=0$. Examining the low-temperature limits, we observe that M tends to a discontinuous behavior as function of J_3, and we therefore turn to a systematic investigation of ground-state properties.

GROUND STATES

For the special case $J_1/J_3=-3$, the magnetic susceptibility diverges at $T=0$, as shown in Fig. 4. Without having the benefit of prior experience with odd-spin clusters, we do not know *a priori* whether the ground-state properties mimic the $T\rightarrow 0$ limit of thermodynamically computed properties. (One-dimensional systems notoriously have their phase transitions, if any, at $T=0$ and—worse—are often

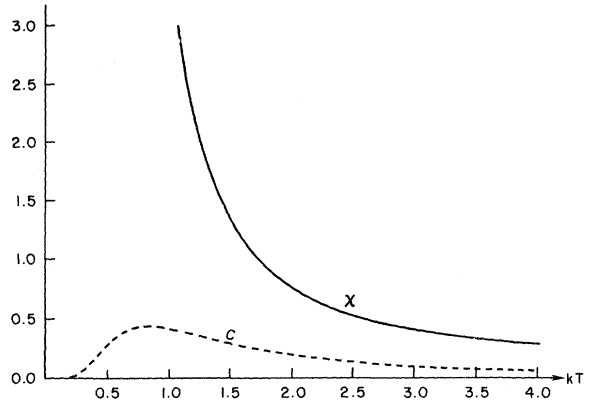

FIG. 2. Specific heat, magnetization, and magnetic susceptibility for $J_1=0, J_3=1$. (Note $M\equiv 0$.)

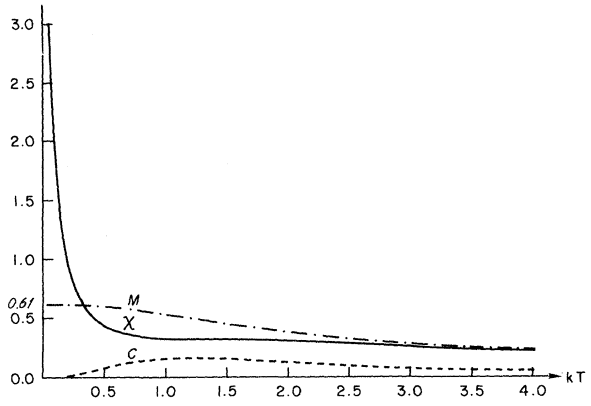

FIG. 4. Same as Fig. 2 for $J_1=-3/\sqrt{10}$, $J_3=1/\sqrt{10}$—the "critical" ratio.

nonergodic, so that delicate questions concerning long-range order may depend on the mode of calculation.) For this special case, and for the general case, we seek to construct the ground state: that configuration (or configurations) which minimizes the energy *per* spin for an infinite chain.

We start by looking for repetition patterns: Each + spin is followed by a number of − spins, etc. Very easily we find the patterns shown in Fig. 7. The notation is obvious: − − − means that cells of three spins have all spins down; − + + (or the two equivalent translations: + − + and + + −) means that in each cell, the spins are down, up, and up. Such a ground state is threefold degenerate, however long the chain may be. The ground-state entropy per spin is thus zero. These results are in general accord with the work of Morita[2] who found that the ground state usually has the periodicity equal to the range of the interactions.

Along the critical line $J_1/J_3=-3$ ($\phi_c=\pi\times 0.897\,58\ldots$) the ground state is no longer so simple. Let $J_1<0$ and $J_3=-\frac{1}{3}J_1>0$. It may be verified that any ground state need merely satisfy the following rules:

Any negative spin is followed by two positive spins; any positive spin immediately preceded by at least one positive spin may be followed by either a positive or a negative spin.

All states satisfying these rules have the same (ground-state) energy. The number of such states W is the ground-state degeneracy, and $\mathcal{S}=L^{-1}k_B\ln W$ is the ground-state entropy *per* spin. We now proceed to calculate this quantity, the average magnetization, and other interesting properties.

Let the chain of length L contain N_1 free spins "up" (+1) and N_2 free spins "down" (−1), thus $N_1+3N_2=L$ at each free spin down is necessarily followed by two spins up. The total number of configurations subject to these rules is the binomial coefficient

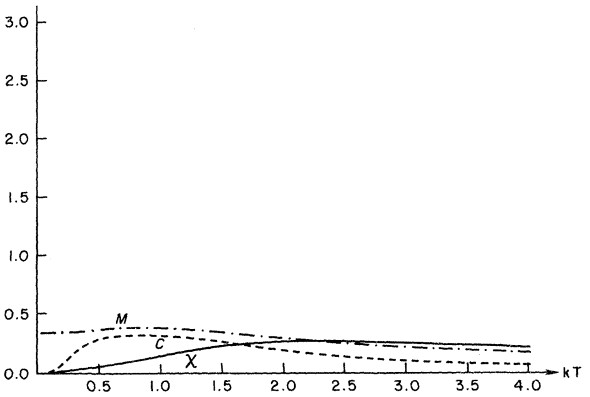

FIG. 3. Same as Fig. 2 for $J_1=-1/\sqrt{2}$ and $J_3=1/\sqrt{2}$.

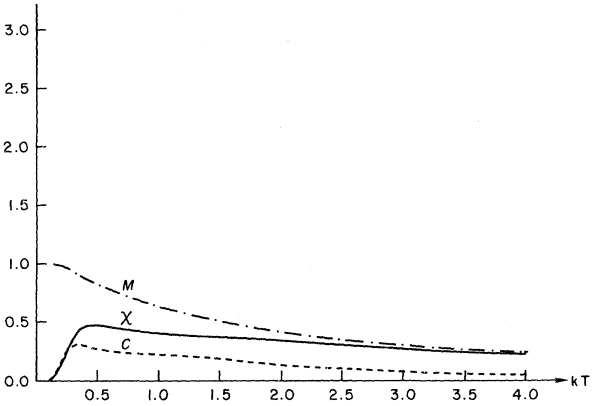

FIG. 5. Same as Fig. 2 for $J_1=-6/\sqrt{37}$ and $J_3=1/\sqrt{37}$.

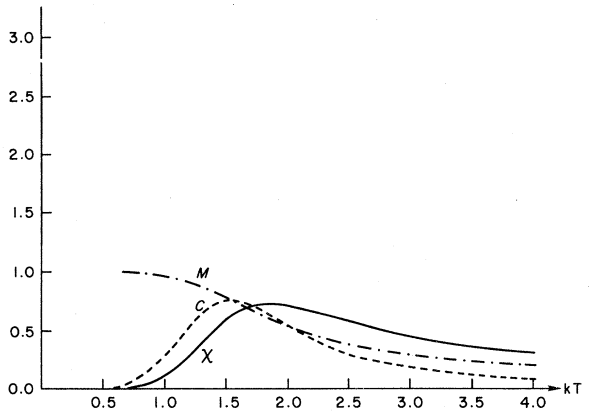

FIG. 6. Same as Fig. 2 for $J_1=J_3=-1/\sqrt{2}$.

$$W(N_2)=\frac{(L-2N_2)!}{N_2!(L-3N_2)!}\ . \tag{7}$$

The optimum N_2 maximizes W, hence

$$W(N_2+1)=W(N_2)[1+O(1/L)]$$

in the thermodynamic (large-L) limit. This condition leads to a cubic equation for $n=N_2/L$:

$$31n^3-31n^2+10n-1=0\ , \tag{8}$$

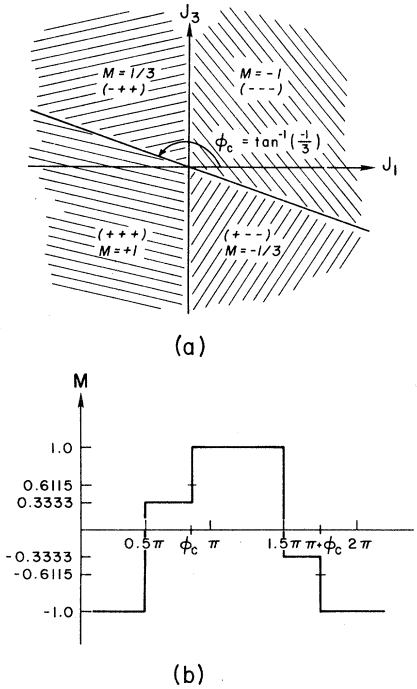

FIG. 7. (a) Phase diagram in (J_1,J_3) plane, indicating magnetization *per* spin M, ground-state configurations, and critical angle ϕ_c. (b) Ground state M as function of angle ϕ in (J_1,J_3) plane, showing discontinuities.

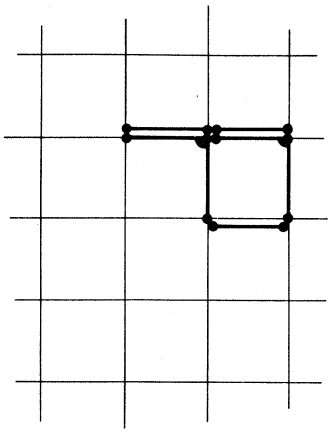

FIG. 8. Lowest-order nonvanishing diagram for binary and ternary (angled) bonds in 2D.

the solution of which is $n=0.19426$. The resultant magnetization *per* spin is

$$M=1-2n=0.6115\ldots\ , \tag{9}$$

which agrees, to the computed accuracy, with the $T=0$ limit of the thermal magnetization, as plotted in Fig. 4. The ground-state entropy is

$$\begin{aligned}\mathcal{S}&=k_B[\,(1-2n)\ln(1-2n)-n\ln n\\&\qquad-(1-3n)\ln(1-3n)]\\&=(0.3823\ldots)k_B\end{aligned} \tag{10}$$

per spin. This is some 55% of the maximum possible entropy $k_B\ln 2$. The number of distinct ground states is approximately $W=(1.446)^L$ out of a total 2^L states. Thus although partially magnetized, the ground state is essentially random or chaotic, as in certain anisotropic nearest-neighbor Ising models.[3] For J_1 positive and $J_3=-\frac{1}{3}J_1$, the average magnetization is $-0.6115\ldots$ but the entropy, an even function, is the same as (10).

HIGHER DIMENSIONS

If H consisted just of stars in two dimensions, as in Fig. 1, it would be written

$$H_{\text{star}}=J_5\sum_n C_n^5\ . \tag{11}$$

Its partition function is trivially calculable because, in the diagrammatic expansion in powers of $\tanh\beta J_5$, no finite length path consisting exclusively of stars can close on itself. Thus only the path of zero length contributes, and Z has the trivial value

$$Z_{\text{star}}=(2\cosh\beta J_5)^N\ , \tag{12}$$

where N equals number of spins. There can be no

phase transition (Z is analytic) nor any long-range order. In three dimensions the partition function calculated from seven-spin star clusters would have exactly the form (12) with J_7 replacing J_5. These "star" partition functions share the features of the special case $J_1=0$ of the preceding section, which one might have been tempted to attribute to the one-dimensional character of that model.

Combining binary and ternary bonds *can* lead to closed paths, as shown in Fig. 8 for J-shaped bonds plus vertical binary bonds. The illustrated diagram has weight $\tanh^2\beta J_3 \tanh^3 \beta J_2$. Evidently, if longer and longer diagrams come to dominate the partition function as T becomes smaller, a phase transition might occur to some kind of ordered phase. (We have not been able to calculate a specific instance of this sort of phase transition as yet). (See note added in proof.)

The Hamiltonian of (11) is not entirely trivial, despite the innocuous Z of Eq. (12). It possesses a large number of ground states. Specifying two rows of a semi-infinite grid causes the third, fourth, and subsequent rows to have their spins oriented uniquely, to minimize the total energy, $-J_5$ for each five-spin cluster. As this can be done for *any* arrangement of spins in the two initial rows, we conclude that the ground-state entropy is $O(N^{1/2})$. Does this imply ground-state order? Certainly, the high-temperature phase is disordered, and we know there is no phase transition. Thus the ground state must be disordered.

PHYSICAL APPLICATIONS

The Ising model was originally intended to explain magnetism, but its greatest successes have been in the study of "lattice gases,"[4] alloys, and the like. In such applications the peculiar symmetry of binary clusters becomes irrelevant, and clusters such as C_n^3 or higher can be significant. This point has been noted recently by others.[5] In magnetic applications, the use of vector spins allows a generalization of the binary Heisenberg interaction to higher clusters such as $\vec{S}_1 \times \vec{S}_2 \cdot \vec{S}_3$. Incredibly, there have been no studies of such interactions in the literature (insofar as we have researched it). Lattice gauge field theories have been constructed in which spin variables are associated with bonds on plaquettes.[6] While plaquettes are usually drawn on hypercubic lattices, thereby involving even powers of the spins, a generalization to triangular of higher odd-coordination lattices would bring, in a most natural way, odd-spin cluster interactions somewhat different from, but related to those we have analyzed in the present work.

Note added in proof. K. A. Penson, R. Jullien, and P. Pfeuty [Phys. Rev. B 26, 6334 (1982)], in an article which has just appeared, have found such an example in a closely related theory.

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