Phase diagram of the "2+4" model in a mean-field approximation without correlations

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A model with two- and four-spin interactions, with coupling constants J_2 and J_4, respectively, is studied using a mean-field approximation without correlations. The phase diagram in the x,T plane ($x=-J_4/J_2$, $J_2>0$, $J_4<0$) possesses three regions, corresponding to a paramagnetic, a ferromagnetic, and a "three spins up and one down" ($\langle 3\,1\rangle$) phase. The transition between the ferromagnetic and the paramagnetic region is second order and independent of J_4. The transition from the $\langle 3\,1\rangle$ to the paramagnetic phase is first order, and its critical temperature is asymptotically linear in x. The discontinuity is shown to be due to the n-spin interaction, and to appear for $n>2$. We have found numerical evidence indicating that incommensurate phases should not appear in the "2+4" model.

I. THEORY

In recent years model Hamiltonians with multispin interactions have been the object of several investigations, due to their possible application to, among other systems, the magnetic structure of ^3He (Ref. 1), NiS_2, and Cu_6Eu (Ref. 2) and, more recently, to lipid bilayers.[3] In addition to the n-spin interaction it may be necessary to consider a second one, of two spins. When both interactions compete with each other the system may present interesting features, such as different phases, possibly including modulated ones, Lifshitz points, infinite-ground-state degeneracy, etc. A great deal of information is contained in a phase diagram where one of the axes is the ratio between the four- and two-spin coupling constants (J_4 and J_2, respectively). For instance, a quantum one-dimensional version of the "2+4" model has been studied by Penson[4] and by Kolb and Penson[5] using finite-size scaling. They found that the phase diagram is similar to that of the axial next-nearest-neighbor interaction (ANNNI) model, except for the absence of a region of incommensurate phases. Also, Grynberg and Ceva[6] have obtained the phase diagram of a two-dimensional "2+4" model, using low- and high-temperature expansions and spin waves. Another debated point is the order of the transition from the ordered to the disordered state, which depends on $x\equiv -J_4/J_2$ and on the number of interacting spins.[7–10] To our knowledge, the determination of the phase diagram in the mean-field approximation (MFA) has not been carried out yet. In spite of its simplicity this method gives, in many cases, results close to the exact ones. In this paper we consider a three-dimensional "2+4" model, applying to it a classical statistical-mechanical formalism in the MFA, without correlations. Our formalism is essentially the same as one that was previously applied to orientational order-disorder transitions.[11–13] In this case there are only two possible orientations, instead of a continuum.

We consider a simple tetragonal lattice where the "2+4" interaction is along the z axis. In the xy plane the spins only interact with the nearest neighbors, with coupling constant J_0. We assume that this interaction is ferromagnetic (FM), and since there is no competition for it, all the spins in the same xy plane are equal to each other in the ground state. Therefore at $T=0$ K the total magnetic energy can be written as

$$H_T=-\sum_i (2J_0S_i^2+J_2S_iS_{i+1}+J_4S_iS_{i+1}S_{i+2}S_{i+3})\,. \tag{1}$$

Here i denotes an xy plane, and the S_i is the spin associated with any of its sites, which can take the values ± 1.

The axial ground-state configurations in the J_2, J_4 plane are shown in Fig. 1. For $J_4>0$ there is no competition and the order is FM for $J_2>0$ and antiferromagnetic (AFM) for $J_2<0$. For $J_4<0$, the four-spin interaction prefers a configuration of the type $\langle 3\,1\rangle$ (we denote a phase of n_1 spins up, n_2 spins down, etc. as $\langle n_1 n_2\cdots\rangle$), whereas the first-neighbor interaction prefers a simple FM or AFM state. The former dominates in the region $|J_4/J_2|>\frac{1}{2}$. From now on, we will assume $J_4<0$.

On the lines $J_4/J_2=\pm\frac{1}{2}$ there exists infinitely many

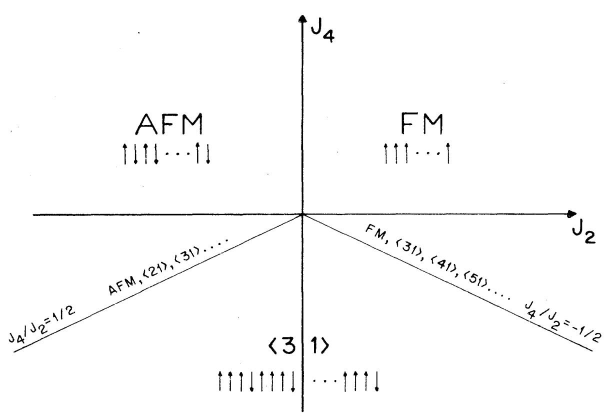

FIG. 1. Diagram of least free-energy configurations at $T=0$ K.

states with the same energy. On $J_4/J_2=\frac{1}{2}$ these states are, in addition to the AFM and the $\langle 3\,1\rangle$, the $\langle 2\,1\rangle$, and those of the form $\langle \cdots n_1 \cdots n_2 \cdots \rangle$, where the n_i are equal to 2 or 3 and the ellipses stand for one or more "1" (for example, $\langle 1\,1\,3\,1\,2\,1\,1\,1\rangle$). For the degenerate states on $J_4/J_2=-\frac{1}{2}$ we can say the following. All the states of the type $\langle n_1 n_2\rangle$, with $n_2\neq 2$, are present. The case of brackets of four or more groups is more complicated, and we do not have a general criterion to decide which ones are present. We have found that phases of the type $\langle n_1 n_2 n_3 n_4\rangle$ with n_2,n_3 equal to 1 or 2 are not present (for example, $\langle 3\,1\,1\,3\rangle$ or $\langle 3\,2\,1\,4\rangle$). Also, configurations $\langle n_1 n_2 n_3 n_4\rangle$ with $n_1>2$, $n_2=1$, $n_3>2$, $n_4=1$ or those with $n_1,n_2,n_3,n_4>2$ are present (for example, $\langle 3\,1\,4\,1\rangle$ or $\langle 3\,3\,4\,3\rangle$, respectively).

Let n_i be the probability that at $T\neq 0$ K a spin of the ith xy plane points in the up direction. We assume that the system has a periodicity of N planes in the z direction (i.e., $n_i=n_{i+N}$, $i=1,2,\ldots,N$). As we wish to express the free energy in terms of one-particle distribution functions, we neglect all correlations between spins (for n-spin interactions with $n>2$ this approximation is stronger than the MFA).

Now the magnetic energy per xy plane takes the form

$$H=-\frac{1}{N}\sum_i (2J_0\langle S_i\rangle^2+J_2\langle S_i\rangle\langle S_{i+1}\rangle +J_4\langle S_i\rangle\langle S_{i+1}\rangle\langle S_{i+2}\rangle\langle S_{i+3}\rangle)\,. \tag{2}$$

In our approximation, the entropy term per plane is

$$S=-(k_B/N)\sum_i [n_i\ln n_i+(1-n_i)\ln(1-n_i)]\,. \tag{3}$$

Instead of n_i, we introduce the average magnetization of the ith layer $M_i\equiv\langle S_i\rangle=2n_i-1$. The free energy $F=H-TS$ is

$$F=-\frac{1}{N}\sum_i\left\{(2J_0M_i^2+J_2M_iM_{i+1}+J_4M_iM_{i+1}M_{i+2}M_{i+3})+\frac{k_BT}{2}\left[M_i\ln\left(\frac{1+M_i}{1-M_i}\right)+\ln\left(\frac{1-M_i^2}{4}\right)\right]\right\}. \tag{4}$$

At a temperature T the distribution functions of the system will be those satisfying the N equations $\partial F/\partial M=0$. This leads to the system

$$M_i=\tanh\{\beta J_0[4M_i+M_{i-1}+M_{i+1}-x(M_{i+1}M_{i+2}M_{i+3}+M_{i-1}M_{i-2}M_{i-3} +M_{i+1}M_{i-1}M_{i-2}+M_{i-1}M_{i+1}M_{i+2})]\}\quad (i=1,\ldots,N)\,, \tag{5}$$

where $x=-J_4/J_2$ and $\beta=1/k_BT$. Here and in the following we assume $J_0=J_2$.

II. RESULTS

In Fig. 2 we show the phase diagram in the x, k_BT/J_0 plane. It presents three phases, in agreement with other authors. Our diagram differs from theirs in that the paramagnetic (PM) region does not extend down to $T=0$ K at $x=0.5$. This difference between the results of mean field and other types of calculations is the same as that existing for the ANNNI model between Bak and von Boehm's[14] and Villain and Bak's[15] phase diagrams, and should be attributed to neglecting correlations.

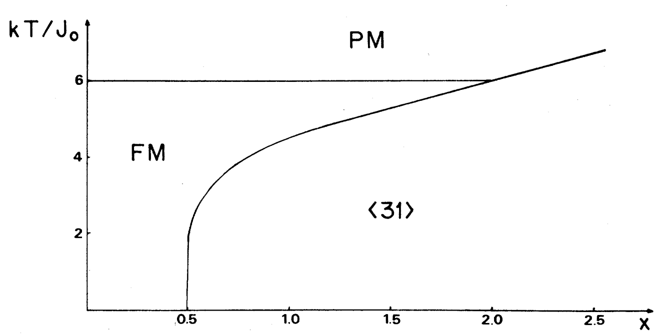

FIG. 2. Phase diagram of the "2+4" model in a mean-field approximation neglecting correlations. Here $x=-J_4/J_2$, with $J_2>0$ and $J_4<0$. We assume $J_0=J_2$.

The transition from the FM to the PM phase is found to be of second order. As just below T_c all the M_i are $\ll 1$, the term with x in (5) can be neglected. So, we conclude that (i) the ordered configuration must be FM as in a simple Ising model, (ii) the transition is independent of the four-spin interaction, and (iii) the critical temperature is $k_0T_c/J_0=6$. The property (ii) has also been found by the first-order perturbation theory.[6]

The transition from the $\langle 3\,1\rangle$ to the PM phase is of first order. The critical line is easily seen to be asymptotically linear in x. In fact, for $x\gg 2$ in the ordered phase all $|M_i|\simeq 1$ and $F\simeq H=-(2+x)J_0$, while in the PM phase $F=-TS=-k_BT\ln 2$. Equating both expressions gives

$$k_BT_c/J_0=\left(\frac{2}{\ln 2}+\frac{1}{\ln 2}x\right). \tag{6}$$

The triple point of the phase diagram is tricritical. Its position is obtained solving system (5) with the condition that the free energy of the $\langle 3\,1\rangle$ phase must be equal to that of the PM phase and imposing $k_BT/J_0=6$. The result is $M_1=M_3=0.936\,388$, $M_2=0.963\,684$, $M_4=-0.887\,389$, and $x=2.006\,042$.

In the $\langle 3\,1\rangle$ region the system (5) has, above a certain temperature (which depends on x), two solutions of the $\langle 3\,1\rangle$ type. The one with the least free energy is that with the larger values of the $|M_i|$, which decrease with increasing temperature; the $|M_i|$ given by the other solution increase with the temperature, and correspond to an

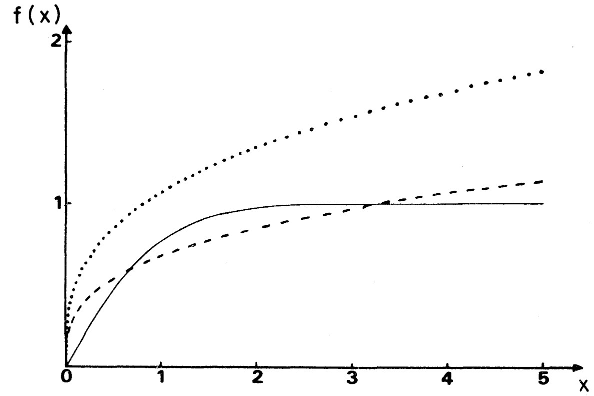

FIG. 3. Graphic solution of Eq. (7). The solid line corresponds to $f(x)=\tanh x$. The dashed (dotted) line corresponds to $f(x)=Ay^{1/(n-1)}$ for $A<(\tau/n)^{1/(n-1)}$ $[A>(\tau/n)^{1/(n-1)}]$. For the sake of definiteness, in this plot we took $n=4$.

unstable situation. Both solutions converge to a single one, but this always happens at a temperature higher than T_c. This behavior is due to the four-spin interaction (see below).

We looked for the existence of modulated phases (here we call "modulated" any phase different from the FM or $\langle 3\,1\rangle$). Our search was carried out near two values of x, where such phases, if they exist, are more likely to be those with the least free energy: $x\simeq 0.5$ and $x\simeq 2.0$. For $x\simeq 0.5$, the modulated phases one should expect are of the type $\langle n\,1\rangle$ $(n=4,5,\ldots)$ (which differ little from the FM for large n and from the $\langle 3\,1\rangle$ for small n), and also $\langle 3\,1\,4\,1\rangle$, $\langle 3\,1\,3\,1\,4\,1\rangle$, ... (which differ little from the $\langle 3\,1\rangle$). We verified that these configurations are solutions to system (5). However, they have a higher free energy than the $\langle 3\,1\rangle$. The same happens for $\langle 3\,3\rangle$, which is one of the most stable configurations in the ANNNI model.[14] A similar thing occurs for $x\simeq 2$. Here, in addition, any modulated phase disappears appreciably before the $\langle 3\,1\rangle$ does, i.e., the latter survives for higher temperatures. The absence of modulated phases occurs because their entropy term is not large enough as to compensate for the loss of the magnetic energy with respect to the $\langle 3\,1\rangle$ configuration. Modulated phases were also looked for by Kolb and Penson,[5] with a negative result. Let us say that our calculations are limited to modulation wavelengths of, at most, 30 sites. However, relying upon our previous arguments, we think that modulated phases should not be expected to be the most stable ones in our MFA.

The behavior of the $\langle 3\,1\rangle$ phase is, to a great extent, due to the four-spin interaction. This can be seen studying the case $J_0=J_2=0$. We do this considering the general case of an n-spin interaction. To fix ideas, let us take $J_n>0$. Now Eq. (5) can be cast into the form

$$M=\tanh(nM^{n-1}/\tau) \quad \text{or} \quad Ay^{1/(n-1)}=\tanh y\,, \qquad (7)$$

with $\tau=k_BT/J_n$, $y=nM^{n-1}/\tau$, and $A=(\tau/n)^{1/(n-1)}$.

For $n=2$ the left-hand side is a straight line, which intersects the hyperbolic tangent at one or no points if $\tau/2<1$ or $\tau/2>1$, respectively. For $n>2$ the left-hand side has an infinite slope at the origin and tends to infinity for $y\to\infty$, so that it can be like the dashed or the dotted line in Fig. 3, depending on the values of n and τ. At low temperature the curve is like the dashed line. As the temperature increases, the two solutions approach each other until coinciding at a certain T, above which they disappear. This gives rise to a discontinuity of the magnetization. Among the two solutions, the one with the greater value of $|M|$ has the lower free energy. The transition to the PM phase occurs when

TABLE I. Values of $\langle M\rangle$ and k_BT/J_n for the interaction of n spins, corresponding to the point of the transition from an ordered to a disordered phase.

n	$\langle M\rangle$	k_BT/J	F/J_n
3	0.948 059	1.487 908	−1.031 339
4	0.990 611	1.451 797	−1.006 309
5	0.997 912	1.444 810	−1.001 457
6	0.999 500	1.443 210	−1.000 357
7	0.999 877	1.442 823	−1.000 088
8	0.999 969	1.442 727	−1.000 022
9	0.999 992	1.442 703	−1.000 006
10	0.999 998	1.442 697	−1.000 001
⋮	⋮	⋮	⋮
∞	1.000 000	1/ln2	−1.000 000

$$-\tau\ln 2=-M^n+\frac{\tau}{2}\left[M\ln\left(\frac{1+M}{1-M}\right)+\ln\left(\frac{1-M^2}{4}\right)\right]. \qquad (8)$$

Equations (7) and (8) form a system whose solutions are presented in Table I.

Let us compare these temperatures with those above which there are only trivial solutions. The latter must satisfy Eq. (7) and

$$\cosh\left(\frac{nM^{n-1}}{\tau}\right)=\left(\frac{n(n-1)}{\tau}\right)^{1/2}M^{(n/2)-1}. \qquad (9)$$

We verified that for any n and J_n these temperatures are higher than those given in Table I. Therefore the transition to the PM phase must occur when there are still two solutions.

This behavior is essentially the same we found in the "2+4" model for the $\langle 3\,1\rangle$ phase so we conclude that it is due to the multispin interaction.

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