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Ordering in a system with finite entropy at $T = 0$

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Abstract. A rigorous Peierls-type proof is given for the existence of a phase transition for an antiferromagnetic Ising model on a CU_3Au lattice with the spins at the gold sites removed. This lattice is known to possess finite entropy at $T = 0$. Thus in contrast to say the planar triangular antiferromagnetic Ising model, which has entropy at $T = 0$ but no phase transition, here is an Ising model which has both.

1. Introduction

Recently Chui (1977) examined an antiferromagnetic Ising model on a Cu_3Au lattice with non-magnetic impurities at the Au sites. He showed that at zero temperature the system possessed a finite entropy per spin, and suggested that an ordered phase may still exist despite this finite entropy at $T = 0$.

Here a Peierls-type argument (Peierls 1936, Griffiths 1964) is used to show rigorously that an ordered phase does indeed exist. Part of the lattice which is to be considered is shown in figure 1. The positions of the spins are shown by crosses and full circles. At the centre of each alternate octet of spins denoted by a cross is another spin denoted by a full circle. Interactions between nearest neighbours are depicted in figure

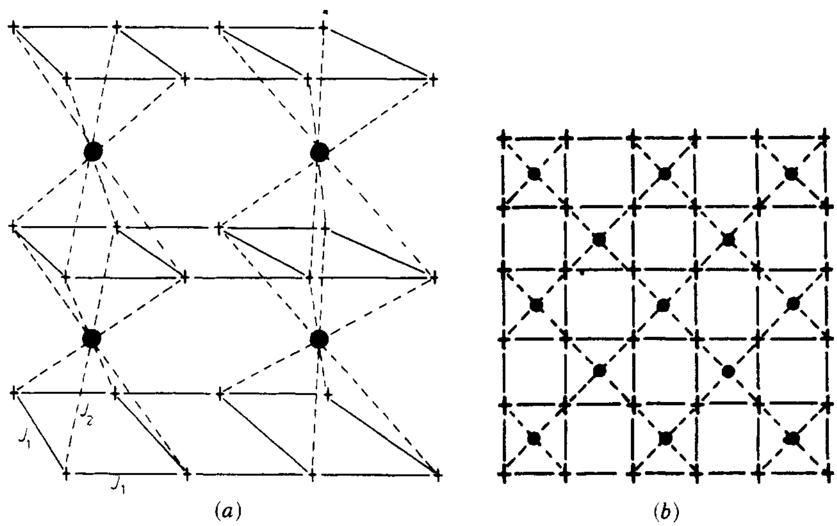

Figure 1. Part of Cu_3Au lattice shown: (*a*) from the side; and (*b*) from above. Spins are depicted by crosses and full circles, and bonds by full and broken lines.

1 by full and broken lines, and the coupling between all spins is taken to be less than zero. It is convenient to divide the spins of the lattice into two sets, denoted by X_1 and X_2 and defined as follows:

(i) The set of spins at the base of the pyramids of the lattice and depicted as crosses in figure 1 belong to set X_1.

(ii) The spins at the tips of the pyramids and depicted by full circles belong to set X_2.

Denote by $\sigma_{x_1} = \pm 1$ and $\sigma_{x_2} = \pm 1$ the spins of X_1 and X_2 respectively. Now each spin interacts with its nearest neighbours only and the energy E of the lattice is

$$E = -J_1 \sum_{\langle x_1 x_1 \rangle} \sigma_{x_1}\sigma_{x_1} - J_2 \sum_{\langle x_1 x_2 \rangle} \sigma_{x_1}\sigma_{x_2} \tag{1}$$

and

$$J_1, J_2 < 0.$$

$\langle x_1 x_1' \rangle$ denote summation over nearest neighbours. The distribution function for any arrangement of the spins is

$$\exp(-\beta E), \qquad \beta = 1/kT.$$

Note that spins in different layers and belonging to X_1 interact only through the spins of X_2. Peierls' (1936) original argument for the existence of a phase transition in the two-dimensional Ising ferromagnet is a powerful geometric argument which in essence bounds the probability of fluctuations from the ground state and from this it is possible to infer the existence of a phase transition. Here, because of the peculiar geometry of the lattice, these bounds cannot be expressed in terms of the length (surface area) of the boundary between regions of opposite order as in the original Peierls' proof. In addition, the ordering can be quite subtle in that it may only be the spins of X_1 which become ordered while the spins of X_2 remain disordered. It is the disorder of X_2 which gives rise to the finite entropy at zero temperature as shown by Chui (1977) and as will arise as a natural consequence of the proof of a phase transition. The nature of the ordering will depend on the ratio J_1/J_2 and can be either antiferromagnetic or ferromagnetic even though J_1, $J_2 < 0$. In fact this lattice can be regarded as having competing order parameters; but discussion of this will be delayed until after the proof has been given. Finally it is noted that there are two-dimensional antiferromagnets which have finite entropy per spin at $T = 0$. The triangular lattice has finite entropy per spin at $T = 0$ but no phase transition (Wannier 1950), while the 'union jack' lattice with a spin at the site of the crossed bands does have a phase transition and can have entropy at $T = 0$ (Vaks *et al* 1965).

Somewhat anticipating the results the calculation is divided into two cases $J_1 \leq J_2 < 0$ and $0 > J_1 > J_2$.

2. Calculation: $J_1 \leq J_2$

For the moment consider X_1 only and impose the following boundary conditions on the sub-lattice which they make up. Let the boundary columns of this sublattice be alternately fixed with positive or negative spins. Let the first and last layers of this sublattice have their spins fixed such that each negative spin is surrounded by positive spins and vice versa. Thus these first and last layers have the perfect antiferromagnetic order. Now sublattice X_1 is partitioned by drawing unit areas on the dual of sublattice X_1 using the following rules:

(i) If two neighbouring spins in the *same* layer of sublattice X_1 are *parallel* then draw a unit area perpendicular to the line joining them and midway between them.
(ii) If two spins in *neighbouring* layers of X_1 are *antiparallel* then draw a unit area midway between them and perpendicular to the line joining them.

In this way sublattice X_1 is partitioned by a set of closed surfaces. Denote the set of such surfaces by B. So far nothing has been said about sublattice X_2 and the above can be carried out without reference to it.

It is well known that, say for a rectangular or cubic lattice, B uniquely identifies the energy of the lattice. This is not the case for the present lattice as the spins of X_2 can take any value without altering B. A lattice with no surfaces will have perfect antiferromagnetic ordering in each layer of X_1 and ferromagnetic ordering in each column. In the Peierls' proof only the area of B is relevant; however, here the number of corners, edges and interactions will be important.

It is important to state clearly what is to be meant by the phrase 'the interaction across B'. By this is meant interaction between all pairs of spins of X_1, one inside B and one outside B, either joined directly by a bond of sublattice X_1 or indirectly via a single spin of X_2. The programme is now to bound the probability of configuration B and from this to infer the existence of a phase transition.

Define:

(*a*) n to be the total surface area of B.
(*b*) n_h and n_v to be the horizontal and vertical components of n.
(*c*) n_1 to be the number of sites of X_2 where there is an intersection between two vertical planes of B (figure 2(*a*)).
(*d*) n_2 to be the number of sites of X_2 where there is a corner of B (figure 2(*b*)).
(*e*) n_3 to be the number of sites of X_2 where there is a vertical edge of B (figure 2(*c*)).
(*f*) n_4 to be the number of sites of X_2 where there is a horizontal edge of B intersected by a plane (figure 2(*d*)).

Knowing the above is all that is required to fix the maximum energy of interaction across B. To see this, note that for a corner edge etc not at a site of X_2, no additional interactions across B are incurred other than those included in (*b*). Further, there is no effective interaction across n_h. This is because the layers of X_1 are connected only through spins of X_2 and the sum of any eight of X_1 separated by horizontal sections of B is zero. Thus there is no net contribution to the energy of the lattice coming from n_h, except possibly from the edges of these horizontal sections and such energy contributions have already been accounted for in n_2 and n_4.

Define N_2 to be the set of unit surfaces of B which meet at the n_2 sites of X_2 where there is a corner of B. Similarly define N_1, N_3 and N_4 for the other types of intersections defined in (*c*), (*e*) and (*f*). Let $E(B)$ be the energy of the lattice which is partitioned by B. Then

$$E(B) \leq -[n_v J_1 - J_2(8n_1 + 2n_2 + 4n_3 + 4n_4)] + E^c(B) \tag{2}$$

or more generally,

$$E(B) = -\left[n_v J_1 - J_2\left(8 \sum_{x_2 \in n_1} \sigma_{x_2} + 2 \sum_{x_2 \in n_2} \sigma_{x_2} + 4 \sum_{x_2 \in n_3} \sigma_{x_2} + 4 \sum_{x_2 \in n_4} \sigma_{x_2}\right)\right] + E^c(B). \tag{3}$$

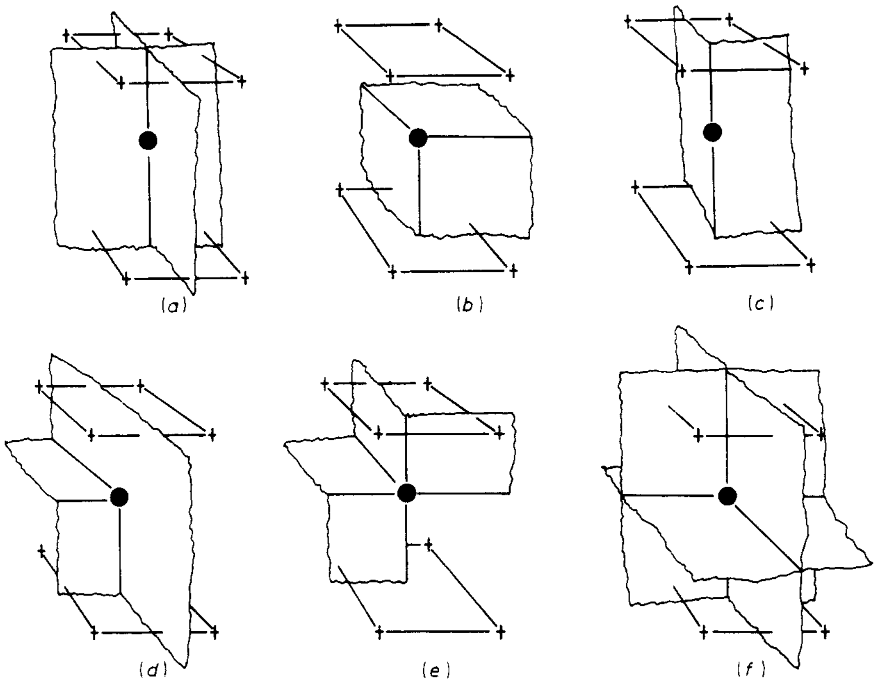

Figure 2. Types of intersections at sites of X_2.

$E^c(B)$ is the contribution to the energy coming from all interactions *not* across B. Hence if $P(B)$ is the probability of configuration B then from (3)

$$P(B)=e^{n_vJ_1\beta}\sum_{(X_2)}{}' e^{-\beta E^c(B)}\frac{(2\cosh 8J_2\beta)^{n_1}(2\cosh 2J_2\beta)^{n_2}(2\cosh 4J_2\beta)^{n_3}(2\cosh 4J_2\beta)^{n_4}}{Z2^{n_1+n_2+n_3+n_4-d}} \tag{4}$$

$$Z=\sum_{(X_1)(X_2)} e^{-\beta E}. \tag{5}$$

d is the number of spins of X_2 which lie on B. Z is the partition function and the summation is over all σ_{x_1} and σ_{x_2} subject to the boundary conditions. $\Sigma'_{(X_2)}$ denotes summation over all spins of X_2 which do not lie on B. A lower bound is constructed for Z by restricting the summation over (X_1) and (X_2) to states in which there are no surfaces at all. Denote the set of such states by G. Then

$$Z\geqslant\sum_G e^{-\beta E}=2^d\, e^{-n_v\beta J_1}\sum_{(X_2)}{}' e^{-\beta E^c(B)}. \tag{6}$$

From (4) and (6) it follows that

$$P(B)\leqslant e^{2n_v\beta J_1}\frac{(2\cosh 8J_2\beta)^{n_1}(2\cosh 2J_2\beta)^{n_2}(2\cosh 4J_2\beta)^{n_3}(2\cosh 4J_2\beta)^{n_4}}{2^{n_1+n_2+n_3+n_4}}. \tag{7}$$

The problem is now to bound (7). The first step is to choose T_1 such that for $T<T_1$

$$e^{\beta J_2}<\eta<1. \tag{8}$$

η is arbitrary but small. Typically η could be chosen to be 10^{-6}; for the moment it does not matter; a suitable choice will be made later. Then

$$P(B) \leqslant \exp\{\beta[2n_v J_1 - 2J_2(4n_1+n_2+2n_3+2n_4)]\}\left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4}. \quad (9)$$

A bound is put on (9) by expressing n_v in terms of n_1, n_2, n_3 and n_4. The type of bound that will be constructed and that will be sufficient for later use will depend on whether $J_1<J_2$ or $J_1=J_2$. Note that each unit area of B can at most belong to two of the sets N_1, N_2, N_3 and N_4 (or the same set twice). This is because of the strange geometry of the lattice. To convince oneself of the truth of the above statement just imagine a unit area which forms part of a corner, then this unit area can at most form part of two corners which are at a site of X_2. Thus a lower bound for n_v is half the total number of vertical unit areas needed to construct n_1 intersections, n_2 corners etc. Thus

$$n_v \geqslant \tfrac{1}{2}(8n_1+2n_2+4n_3+6n_4), \quad (10)$$

and from (9) and (10) it follows that

$$P(B) \leqslant \exp[2\beta n_v(J_1-J_2)]\left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4}. \quad (11)$$

This bound is sufficient for $J_1 \neq J_2$. For $J_1=J_2$ write

$$4n_1+n_2+2n_3+2n_4 = n_v - b, \qquad b \geqslant 0. \quad (12)$$

It follows that

$$n_1+n_2+n_3+n_4 \geqslant \tfrac{1}{4}n_v - \tfrac{1}{4}b. \quad (13)$$

Thus from (9),

$$P(B) \leqslant \exp(2J_1\beta b)\left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4} \quad (14)$$

It is now possible to show that for sufficiently low temperatures an ordered state can exist. To do this the correct order parameter must be chosen and bounded strictly greater than zero. Now

$$x_1 = (i, j, k) \qquad i, j, k = 1, 2, \ldots$$

and define

$$m_1 = \frac{1}{V}\sum_{(X_1)} \sigma_{x_1}(-1)^{i+j} \quad (15)$$

with V the number of spins of X_1. Then

$$\lim_{V\to\infty}\langle m_1\rangle \geqslant \lim_{V\to\infty}\left(1-\frac{2}{V}\sum_B V(B)D(B)P(B)\right). \quad (16)$$

$V(B)$ is the number of spins inside B and $D(B)$ can be defined as follows: split B into a maximal set of connected components $B_1, B_2, \ldots, B_r$ which shall be called cycles†.

† The word 'cycles' is used here in a slightly different sense to Ruelle. In Ruelle (1969) 'cycles' are defined in such a way as to have no intersections. Here the restriction on intersections is dropped. This is why it is possible to construct a tighter bound on the number of connected components of B than the one in Ruelle (1969).

Then $D(B)$ is the number of cycles with the prescribed number of crossings and corners etc as defined earlier. A bound on $D(B)$ can be constructed in much the same way as Griffiths (1964) and Ruelle (1969) with a few modifications. If there were no knowledge about the number of corners, crossings etc then a bound could be constructed as in Ruelle (1969) to give

$$V3^{n_v-1}.$$

The 3^{n_v-1} comes from the requirement that each unit area can be added in one of three ways. However, knowing that there are n_1 crossings etc reduces the degree of freedom of those unit areas involved in constructing these intersections etc to one. Hence from (10) the following is found:

$$D(B) \leqslant V3^{n_v-(4n_1+n_2+2n_3+3n_4)}. \tag{17}$$

For $J_1 < J_2$

$$\lim_{V\to\infty} \langle m_1 \rangle \geqslant 1 - \sum_B V(B) 3^{n_v-(4n_1+n_2+2n_3+3n_4)} \left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4} \exp[2\beta n_v(J_1-J_2)]. \tag{18}$$

A sufficient bound for $V(B)$ for the present is

$$V(B) \leqslant (n_v/4)^{3/2}. \tag{19}$$

Then the second term of (18) is less than or equal to

$$\sum_{n_v=4}^{\infty} 2\left(\frac{n_v}{4}\right)^{3/2} \left(\frac{1+\eta}{2}\right)^{n_v} 3^{n_v} e^{2\beta n_v(J_1-J_2)} = \alpha_1(T).$$

In particular the above series is convergent and can be bounded as small as is pleased. Then choose $\alpha_1(T) < 1$ for $T < T_{c_1}$. Then

$$\lim_{V\to\infty} \langle m_1 \rangle > 1 - \alpha_1(T) > 0 \qquad \text{for } T < T_{c_1}. \tag{20}$$

Hence there is an ordered phase for $T < T_{c_1}$ and $J_1 < J_2$. There is also a phase transition for $J_1 = J_2$ but the proof is a little more involved. Using (14), (16) and (17), then for $J_1 = J_2$

$$\lim_{V\to\infty} \langle m_1 \rangle \geqslant 1 - \left[2 \sum_B V(B) 3^{n_v-(4n_1+n_2+2n_3+3n_4)} \left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4} e^{2J_1\beta b} \right]. \tag{21}$$

The summation in (21) is divided into two parts: a summation for which $b \neq 0$ and a summation for which $b = 0$. The second term of (21) becomes

$$2 \sum_{\substack{B \\ b\neq 0}} V(B) 3^{n_v-(4n_1+n_2+2n_3+3n_4)} \left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4} e^{2J_1\beta b}$$
$$+ 2 \sum_{\substack{B \\ b=0}} V(B) \left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3+n_4} 3^{n_v-(4n_1+n_2+n_3+3n_4)}. \tag{22}$$

The first of these terms can be easily disposed of. Use (13) and (12) to write the first term of (22) as less than or equal to

$$2 \sum_{\substack{B \\ b\neq 0}} V(B) \left(\frac{1+\eta}{2}\right)^{n_v/4} \left[3 \left(\frac{1+\eta}{2}\right)^{-1/4} e^{2\beta J_1} \right]^b. \tag{23}$$

(19) is again a sufficient bound for $V(B)$. Hence (23) becomes less than or equal to

$$3\left(\frac{1+\eta}{2}\right)^{-1/4} e^{2\beta J_1} \sum_{n_v=4}^{\infty}\left(\frac{n_v}{4}\right)^{3/2}\left(\frac{1+\eta}{2}\right)^{n_v/4}, \tag{24}$$

where T is chosen sufficiently small to make $3[(1+\eta)/2]^{-1/4} e^{2\beta J_1}<1$. Now the series in (24) is convergent by the ratio test remembering that $\eta<1$. Hence by choosing T small, (24) can be bounded as small as is pleased. Define (24) to be

$$\alpha_2(T) \underset{T\to 0}{\to} 0. \tag{25}$$

The second term of (22) is slightly harder to bound as there are no exponentially small factors to control the growth of the series. In fact, it is obviously not possible to bound this series to zero as $T\to 0$ as in the previous two series. It is necessary to carefully take into account the consequences of $b=0$ which are as follows:

$$b=0 \quad\Rightarrow\quad n_4=0, \tag{26a}$$

$$b=0 \quad\Rightarrow\quad n_v=4n_1+n_2+2n_3, \tag{26b}$$

$$b=0 \quad\Rightarrow\quad V(B)=n_v/4. \tag{26c}$$

Using (26) in the second term of (22) yields

$$2\sum_B\left(\frac{1+\eta}{2}\right)^{n_1+n_2+n_3}\left(n_1+\frac{n_2}{4}+\frac{n_3}{2}\right). \tag{27}$$

Before summing (27) it must be noted that $n_1\neq 0\Rightarrow n_2\geq 4$ and $n_3\geq 2$, and $n_3\neq 0\Rightarrow n_1\geq 4$. So (27) is bounded above by

$$2\left[\left(\frac{1+\eta}{2}\right)^6\sum_{n_1\geq 1}^{\infty}\left(\frac{1+\eta}{2}\right)^{n_1} n_1+\frac{1}{4}\sum_{n_2\geq 4}^{\infty}\left(\frac{1+\eta}{2}\right)^{n_2} n_2+\frac{1}{2}\left(\frac{1+\eta}{2}\right)^4\sum_{n_3\geq 2}^{\infty}\left(\frac{1+\eta}{2}\right)^{n_3} n_3\right]. \tag{28}$$

η can be chosen as small as is pleased by choosing T_1 small enough, as can be seen from equation (8). Let

$$\eta\simeq 10^{-3} \qquad T<T_1.$$

Hence (28) sums to

$$\tfrac{1}{2}+O(10^{-3}). \tag{29}$$

From (21), (22), (25) and (29) it follows that for $J_1=J_2$

$$\lim_{V\to\infty}\langle m_1\rangle \geq 1-\alpha_2(T)-\tfrac{1}{2}-O(10^{-3})\geq \tfrac{1}{2}-\alpha_2(T)-O(10^{-3}). \tag{30}$$

For $T<T_{c_2}, \alpha_2(T)<\frac{1}{4}$. (30) also holds when $J_1<J_2$. However, the bound already constructed for this case and given by (20) shows that the system saturates at $T=0$. From (30) it follows that for $T<\min(T_1, T_{c_2})$

$$\lim_{V\to\infty}\langle m_1\rangle>0.$$

Equations (20) and (30) yield the required result that for all $J_1\leq J_2$

$$\lim_{V\to\infty}\langle m_1\rangle>0 \qquad \text{for } T<\min(T_1, T_{c_1}, T_{c_2})>0. \tag{31}$$

An ordered state has been proved to exist and hence from general thermodynamic considerations the system has been shown to undergo a phase transition. The order parameter has been identified and is given by (15). This order parameter describes the ordering of the spins of sublattice X_1. The ordered phase has antiferromagnetic ordering in the planes of X_1 and ferromagnetic ordering in the columns. For $J_1 < J_2$ and $T = 0$ the order parameter saturates, as can be seen from (20). In this state the spins of X_2 are essentially free giving an entropy per spin at $T = 0$ of

$$\lim_{V\to\infty} \frac{2}{3V} \ln(2^{V/2}) = \frac{1}{3} \ln 2. \tag{32}$$

For $J_1 = J_2$ the system will have this characteristic ordering given by order parameter of equation (15). However, the entropy per spin can be shown to be strictly greater than (32). Hence for $J_1 = J_2$ the order parameter does not saturate at $T = 0$. For $J_1 < J_2$ and at $T = 0$, and *only* then, the correlation between the neighbouring layers of X_1 breaks down.

3. Calculation: $J_2 < J_1 < 0$

None of the bounds constructed in § 2 hold for $J_2 < J_1 < 0$. It will now be shown that for sufficiently small temperatures a different type of ordering occurs. In this case all boundary spins of X_1 are made positive and the lattice is partitioned by drawing unit areas on the dual of X_1 between any neighbouring spins of X_1 which are antiparallel. This partitions the lattice by closed surfaces; call the set of such surfaces C. These surfaces intersect themselves and again the energy of a given configuration C will depend on the number and type of intersections, though not in the same way as before. Define:

(*a*) n to be the total area of C.
(*b*) n_v and n_h to be the vertical and horizontal component of n.
(*c*) l_1 to be the number of sites of X_2 where there is an edge of C (figure 2(*c*)).
(*d*) l_2 to be the number of sites of X_2 where there is a corner of C (figure 2(*b*)).
(*e*) l_3 to be the number of sites of X_2 where there are two corners of C (figure 2(*e*)).
(*f*) l_4 to be the number of sites of X_2 where there is an intersection of two planes of C (figure 2(*a*)).
(*g*) l_5 to be the number of sites of X_2 where three planes of C intersect (figure 2(*f*)).
(*h*) l_6 to be the number of sites of X_2 where there is an intersection of an edge and a plane of C (figure 2(*d*)).

Denote by L_1 the set of unit areas which meet at the l_1 sites of X_2 where there is an edge of C. Define L_2, L_3, L_4, L_5 and L_6 similarly. Note that even though the same diagrams have been used to illustrate (*c*), (*d*), (*f*) and (*h*) of the above there are slight differences in some of these definitions from those that were used before. For example in (*f*) it is no longer required that the planes should be vertical. Denote by $E(C)$ the energy of the lattice which is partitioned by C:

$$E(C) \leq n_v J_1 + J_2(4l_1 + 6l_2 + 4l_3) + E^c(C). \tag{33}$$

$E^c(C)$ comes from all interactions not across C. Then the probability of C is thus

$$P(C) \leqslant 2^n \frac{\exp\{-\beta[n_v J_1 + J_2(4l_1 + 6l_2 + 4l_3)]\}}{Z} \sum_{(X_2)}{}' e^{-\beta E^c(C)} \tag{34}$$

Z is the partition function which is the sum over all $\sigma_{x_1}, \sigma_{x_2}$ subject to the boundary conditions. This summation is restricted to states such that there are no surfaces present. This is equivalent to just taking configuration C and reversing all spins inside it. Also restrict all spins of X_2 which formerly lay on the surface C to be fixed negative. Denote this state by G and the energy of any state of G by $E^*(C)$. Then

$$Z > \sum_{(X_2)}{}' e^{-\beta E^*(C)}$$

and

$$E^*(C) = -[n_v J_1 - 8J_2(l_1 + l_2 + l_3 + l_4 + l_5 + l_6) \\ - J_2(4n - 8l_1 - 6l_2 - 12l_3 - 16l_4 - 24l_5 - 16l_6)] + E^c(C). \tag{35}$$

(35) can be explained as follows. Nearest-neighbour spins of X_1 formerly separated by C, are now both positive, giving rise to an energy contribution of $-n_v J_1$. The second term of (35) arises because each of the spins of X_2 which belong to one of the sets l_1, l_2, l_3, l_4, l_5 or l_6 is now surrounded by eight positive spins thus giving the second term of (35). Now, if there had been no intersections nor edges of any type in C, then reversing all spins inside C and fixing negative all spins of X_2 which formerly lay on C gives a contribution to the energy of $4nJ_2$. But because there are corners, edges etc this result counts some bonds more than once. The effect of counting bonds more than once is accounted for by subtracting the appropriate number of bonds and this is done in the third term of (35). The last term is the contribution from all other interactions. (35) and (34) yield

$$P(C) \leqslant 2^n \exp[\beta(-2n_v J_1 + 2J_2(2n - 2l_1 - 2l_2 - 4l_3 - 4l_4 - 8l_5 - 4l_6)]. \tag{36}$$

In the same way as before the following bound on n is constructed:

$$n \geqslant 2l_1 + \tfrac{3}{2}l_2 + 3l_3 + 4l_4 + 6l_5 + 4l_6 \\ = 2l_1 + 2l_2 + 4l_3 + 4l_4 + 8l_5 + 4l_3 - (\tfrac{1}{2}l_1 + l_3 + 2l_5). \tag{37}$$

(36) and (37) yield

$$P(C) \leqslant 2^n \exp\{\beta[-2n_v J_1 + 2J_2(n - \tfrac{1}{2}l_1 - l_3 - 2l_5)]\}. \tag{38}$$

It is now possible to demonstrate that an ordered phase exists at low enough temperatures.

Define

$$m_2 = \frac{1}{V} \sum_{X_1} \sigma_{x_1}. \tag{39}$$

Then

$$\lim_{V\to\infty} \langle m_2 \rangle \geqslant \lim_{V\to\infty} \left(1 - \frac{2}{V} \sum_C V(C) D(C) P(C)\right). \tag{40}$$

Sufficient bounds on $V(C)$ and $D(C)$ are

$$\begin{aligned} V(C) &\leqslant (n_v/4)^{3/2}, \\ D(C) &\leqslant V3^{n_v}. \end{aligned} \tag{41}$$

(36) and (38) in (40) yields

$$\lim_{V\to\infty}\langle m_2\rangle \geqslant 1-2\sum_C (n_v/4)^{3/2}3^{n_v}2^n \exp\{\beta[-2n_vJ_1+2J_2(n-\tfrac{1}{2}l_1-l_3-2l_5)]\}. \tag{42}$$

It is not clear at this stage that the last term of (42) can be bounded less than one since the 2^n might be bigger than the exponential. However, this is not so. Write

$$n = n_v + (n_h - \tfrac{1}{2}l_1 - l_3 - 2l_5) + (\tfrac{1}{2}l_1 + l_3 + 2l_5). \tag{43}$$

Then (42) becomes

$$\begin{aligned} 1-2\sum_C &\{(n_v/4)^{3/2}6^{n_v}2^{\frac{1}{2}l_1+l_3+2l_5}\exp[2\beta n_v(J_2-J_1)]\} \\ &\times\{2^{n_h-\frac{1}{2}l_1-l_3-2l_5}\exp[2\beta J_2(n_h-\tfrac{1}{2}l_1-l_3-2l_5)]\}. \end{aligned} \tag{44}$$

Now

$$n_h - \tfrac{1}{2}l_1 - l_3 - 2l_5 \geqslant 0, \tag{45}$$

and hence the expression in the second set of brackets of (44) can be bounded less than or equal to one for $T < T_0$. Also if l_h is the length of the perimeter of the horizontal surfaces, then

$$\tfrac{1}{2}l_1 + l_3 + 2l_5 \leqslant l_h \leqslant 2n_v. \tag{46}$$

Thus, for $T < T_0$, (44) becomes greater than or equal to

$$1-2\sum_{n_v=4}^{\infty}(n_v/4)^{3/2}6^{n_v}2^{2n_v}\exp[2n_v\beta(J_2-J_1)]. \tag{47}$$

For $J_2 < J_1$ the sum in (47) can be bounded as small as is pleased. In particular it can be bounded strictly less than one for $T < T_c$. Hence it has been proved that

$$\lim_{V\to\infty}\langle m_2\rangle > 0 \qquad \text{for } T < \min(T_0, T_c) > 0. \tag{48}$$

Hence an ordered phase exists for $J_2 < J_1$, the order parameter being given by (39), and hence from general thermodynamic principles a phase transition has been proved to exist. Order parameter (39) describes ferromagnetic ordering on X_1. From (47) it can be seen that the order parameter saturates at $T = 0$. Thus all spins of X_1 will be up and this implies that all spins of X_2 will be frozen down, there is no $T = 0$ entropy. In effect for $J_2 < J_1$ the entire system is a ferrimagnet with a perfect groundstate with two-thirds of the spins positive and one-third negative.

4. Conclusion

An ordered phase has been shown to exist and the order parameter has been identified in the two cases $J_1 \leqslant J_2$ and $J_1 > J_2$. A schematic graph of transition temperature as a function of J_2/J_1 is shown in figure 3. The full curves represent the calculated lower bounds on the transition temperature. Now the chain curves representing the true transition temperature must meet at a three-phase point as shown in figure 3. It would be interesting to know if the three-phase point occurs at $T > 0$ or not. The answer to this question seems at the moment beyond the reach of the simple argument used here. The results of a mean field calculation (M A Moore and A Bray 1977, private communication) indicate that the three-phase point does occur at a non-zero temperature. However, since mean field calculation give upper bounds this result is not conclusive.

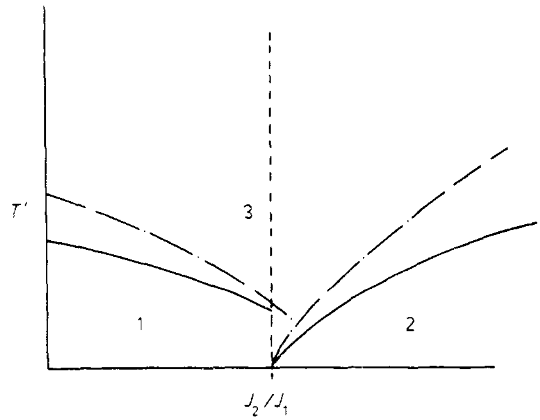

Figure 3. Transition temperature as a function of J_2/J_1 (schemantic). Full curves, calculated bound; chain curves, actual critical temperature. Regions 1, 2 and 3 are antiferromagnetic, ferrimagnetic and disordered regions respectively.

It is possible to perform a partial trace over the spins of X_2. Doing this leaves the lattice X_2 with two, four and eight spin ferromagnetic interactions between different layers of X_2. This is why the system can be regarded as having competing order parameters due to the antiferromagnetic coupling within the layers of X_1 and the ferromagnetic coupling between the layers of X_1.

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