PHYSICAL REVIEW B VOLUME 15, NUMBER 1 1 JANUARY 1977

Simple three-dimensional Ising model with finite entropy at zero temperature

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(Received 15 April 1976)

I show rigorously that an antiferromagnetic Ising model (with only nearest-neighbor interactions) on a Cu_3Au lattice with spins at the gold sites removed possesses finite entropy at zero temperature. I furthermore propose that an ordered phase exists and that the zero-point fluctuation does *not* destroy this order.

I. INTRODUCTION

It is well known that the ground state of the planar triangular antiferromagnetic Isling lattice with nearest-neighbor interaction is so degenerate that entropy consideration always dominates at a finite temperature and *no* magnetic ordering takes place.[1] The fcc antiferromagnetic Ising lattice, which can be viewed as a stack of "triangular Ising" planes with normals pointing in the [111] direction, does go through a magnetic phase transition despite the fact that the ground state is infinitely degenerate, as is shown by Danielian.[2] The total number of ground states is of the order of $2^{0.5N^{2/3}}$, where N is the total number of spins present; the entropy per particle therefore goes like $N^{-1/3}$ and approaches zero as N approaches ∞. If we remove some of the spins from the fcc lattice, interplanar coupling will decrease; the ground-state degeneracy will increase. It may then be possible to achieve a state with finite entropy per particle and no magnetic ordering even though the lattice is still three dimensional. I found that for some rather simple three-dimensional lattices the entropy per particle does become finite; however, an ordered phase may still be possible in these situations.

These fcc lattices are illustrated in Figs. 1–3 with spins at the positions indicated by the circles removed. In particular, the lattice shown in Fig. 3 corresponds to the Cu_3Au lattice with the nonmagnetic impurities at the Au sites.

I shall show in Sec. II rigorously that the entropy per particle is indeed finite and then point out in Sec. III why these degeneracies will only reduce, but not eliminate, the average value of the order-parameter correlation function.

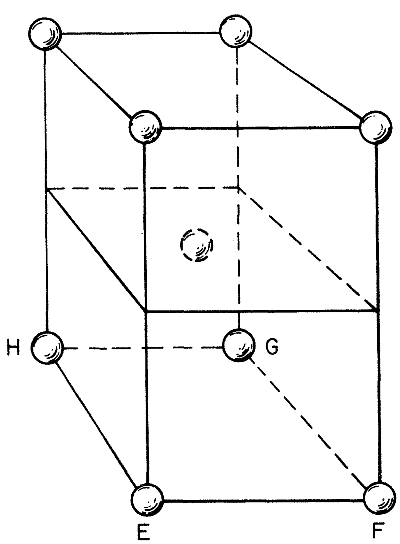

FIG. 1. Primitive cell of the superlattice when impurities are put in. The circles indicate the positions of the nonmagnetic impurities. The magnetic spins are situated at the lattice sites and are not shown.

II. THE GROUND STATES AND ITS ENTROPY

The form of the ground state and its degeneracy is the subject matter of this section. My argument will apply to the situations in Figs. 1–3 but I shall restrict my attention to lattice 2. My argument is similar to that of Danielian[2] and is strongly influenced by his. The general philosopy is to decompose the lattice into basic building blocks, enumerate all possible lowest-energy spin ar-

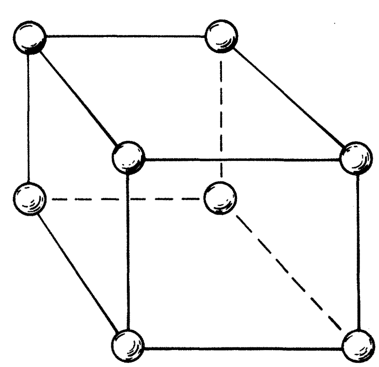

FIG. 2. Another possible primitive cell for another superlattice. Again, the circle denotes the position of the nonmagnetic impurity.

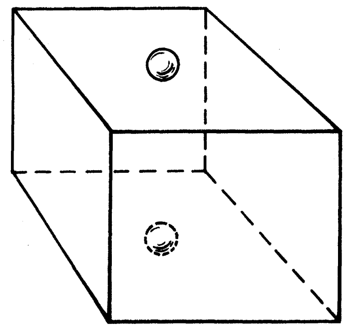

FIG. 3. Another possible primitive cell for another superlattice. Again, the circle denotes the position of the nonmagnetic impurity.

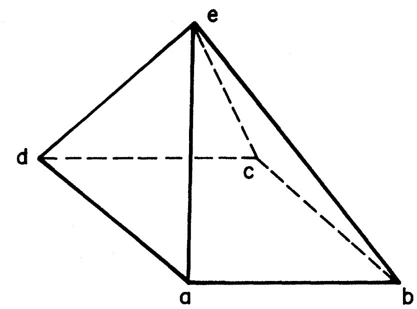

FIG. 5. Side view of the pyramid. Only the pyramid pointing upwards is shown. The corresponding one pointing downwards is not shown here.

rangements for these blocks, and finally show that these arrangements can be put back together on the lattice. Let us look at Fig. 4 where we have drawn a projection of the lattice in the $[0,0,1]$ direction. The crosses indicate spins at the face-center positions $(0,a/2,a/2)$, etc. The squares indicate atoms at the cube corners, E,F,G,H (see Fig. 1). Consider a pyramid with a square base (*abcd*) as is indicated in both Figs. 4 and 5. These pyramids constitute a basic building block of the lattice; each of the bonds on the base (*abcd*) is shared with a neighbor while the bonds on the sides (*ae*, *be*, *ce*, *de*) belong to the pyramid alone. If the energy of each pyramid is minimized then the total energy is also minimized. We first find how many possible arrangements there are and then show that it is indeed possible to put these arrangements together.

Figure 6 is a top view of the basic pyramid and shows all the possible lowest-energy states. It consists of situations with 4, 3, and 2+ spins on the base (we have not shown the corresponding situation with the positive spins replaced by the negative spins). This indicates that the lowest energy block is of energy $-2J$ and the only situation not allowed is as illustrated in Fig. 6(c). One can also put these squares together. A typical situation is shown in Fig. 7 where circles represent one layer above and triangles represent one layer beneath. Some other possibilities are illustrated in Figs. 8 and 9. Indeed the lowest-energy states can be achieved. It is also amusing to point out that, with the arrangement in Fig. 7, we can prove that the system possesses a finite entropy per particle at absolute zero. This is because each spin in a circle site can be up or down. The number of possible ground states is thus larger than $2^{N/3}$ where N is the total number of spins. Thus $S/N > \frac{1}{3} ln 2$.

Note, however, that corresponding to the situation in Fig. 7, there is actually long-range order; the spins on alternate layers are arranged just like a planar antiferromagnetic square lattice. There are, of course, other ground states for which this order is destroyed (Figs. 8 and 9, for example). The crucial question is whether the importance of such states outnumber the present one or not. To put it quantitatively, let us look

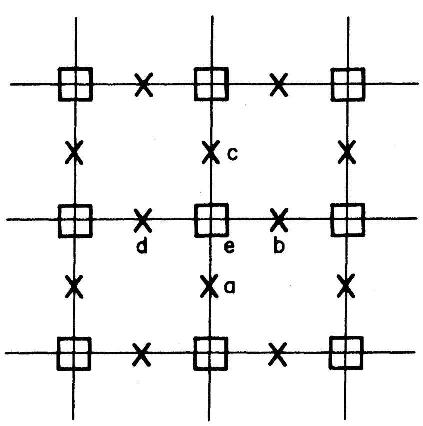

FIG. 4. (001) projection of the basic lattice. The crosses indicate positions at the face-center positions $(0,a/2,a/2)$, etc. A base for a basic pyramid is indicated by *abcd*, with *e* as its tip. Positions indicated by squares are occupied by spins one layer below at $(x,y,0)$. The lattice then repeats itself.

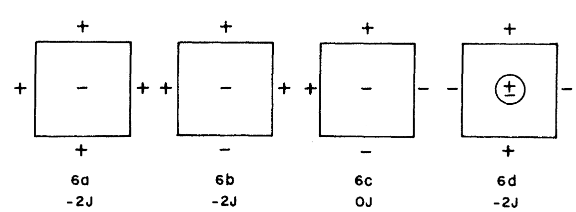

FIG. 6. All the possible spin combinations on a base of a pyramid. The spin in the middle corresponds to that of the tip of a pyramid from either one layer above or one layer below. The corresponding combinations with the "+"'s replaced by the "−"'s, are not shown.

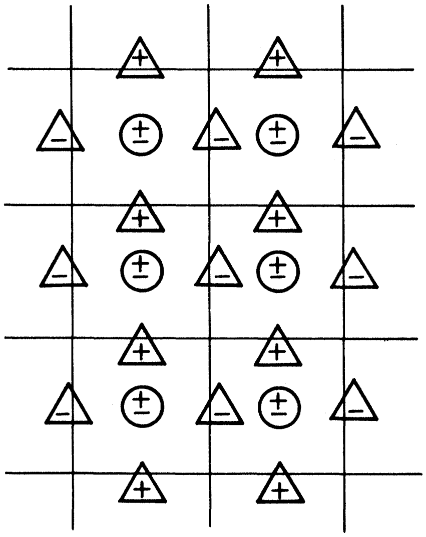

FIG. 7. One possible set of ground-state configurations. Note that the spins in the circle (one layer above) can be either "+" or "−" so that the degeneracy of this state is $2^{N/4}$ where N is the total number of spins.

at the correlation function Δ defined by

$$\Delta = \lim_{\substack{j\to\infty \\ k\to\infty}} \langle S(\vec{r} = 2l\hat{z}) s(\vec{r}' = 2j\hat{x} + 2k\hat{y} + 2l\hat{z}) \rangle,$$

where angular brackets denote thermal averages. The ground-state average value of Δ is given by

$$\Delta = n_1 S^2/(n_1 + n_2),$$

where n_1 is the number of states with a nonzero Δ and n_2 is the number of states for which the order is destroyed. If n_1/n_2 approaches zero (a finite constant) as $N \to \infty$ then the order is destroyed (retained). We have not been able to settle this question rigorously. Instead in the next section we shall give arguments indicating why we think such an order is possible.

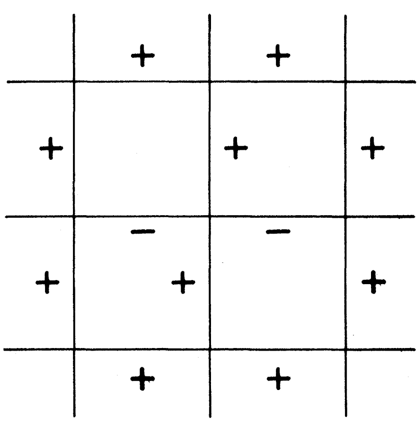

FIG. 8. Another possible ground-state configuration.

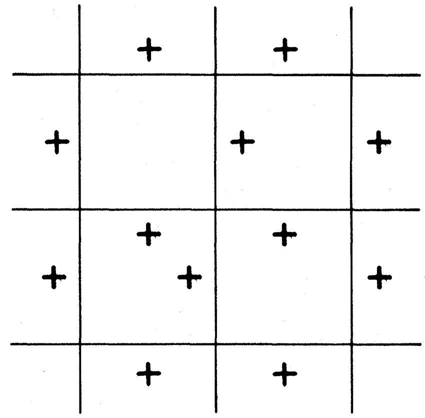

FIG. 9. Another possible ground-state configuration. Only the configuration of the base of the pyramids is shown. The spin arrangement of the tips can be easily put in if one uses the choices in Fig. 6.

III. EXISTENCE OF LONG-RANGE ORDER

The simplest way by which we can flip the spin B at the site $2j\hat{x} + 2k\hat{y} + 2l\hat{z}$ and hence destroy the long-range order is to align its neighboring spins on the upper and lower layer so that they point opposite to those on the same layer; thus allowing spin B to move freely. This gives a contribution to n_2 equal to $\frac{1}{4}n_1$ and will not outweigh the order state. Let us write $n_2 = \sum_i n_2^{(i)}$, where the superscript i indicates various possible spin arrange-

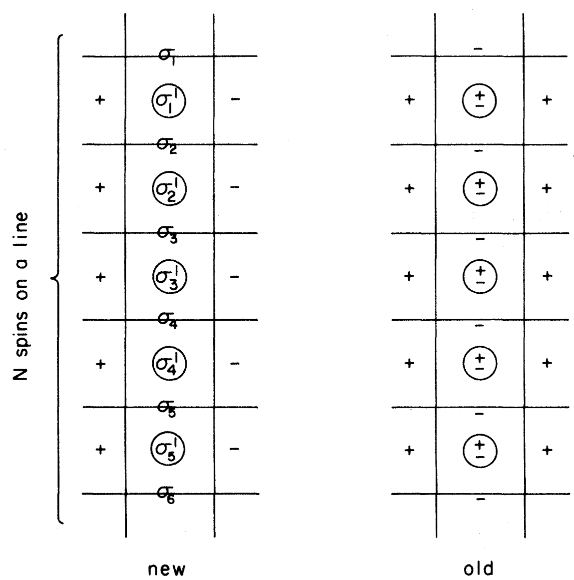

FIG. 10. Graph showing the spin arrangements on a domain wall. The graph on the right-hand side is a section of the regular lattice shown here for comparison. The graph on the left-hand side shows the domain wall.

ments for which the long-range order is destroyed. We thus have $n_2^{(1)} = \frac{1}{4} n_1$.

From the above argument we see that so long as there is long-range order among the spins on the basal planes of the pyramids, the fluctuation of the spins on the tips will not drown out the order. The simplest way to randomize the basal plane spins is to create a domain boundary as is indicated in Fig. 10. On the right-hand side of this figure we have shown the spin arrangements characteristic of our states; on the left-hand side we have shown the simplest boundary we can think of. In order that the spin arrangements conform to either one of Fig. 6(a), 6(b), or 6(d), only two situations are possible, corresponding to $\sigma_1 = \sigma_2 = \sigma_3 \cdots = +, \sigma_1' = \sigma_2' = \cdots = -$ or $\sigma_1 = \sigma_2 = \cdots = -, \sigma_1' = \sigma_2' = \cdots = +$. By creating a domain boundary, the spins σ_1' are no longer free to move. The contributions of this spin arrangement to n_2 is given by $n_2^{(2)} = 2^{-2N+1} n_1 N$. The factor of N comes from the different places at which the domain can be situated. The above number is too small to be of significance. The philosophy of the argument is now clear. Each time we randomize the spins on the basal plane, the spins on the tips will become fixed; the resulting factor overcompensates the entropy of the boundary location. This thus completes our argument in favor of the ordered state.

IV. CONCLUSION

There exist the ice models[3] that possess finite entropy and yet long-range order. These are, however, two dimensional. The present one is three dimensional and still quite simple. It would be interesting to investigate a possible relationship between them.

ACKNOWLEDGMENTS

I thank P. W. Anderson, P. A. Lee, B. I. Halperin, and T. M. Rice for helpful conversations. This work was begun while I was at Bell Laboratories. I should like to thank the hospitality of the theory group there.

*Research partially supported by the SUNY Research Foundation.

[1]G. H. Wannier, Phys. Rev. 79, 357 (1950).

[2]A. Danielian, Phys. Rev. Lett. 6, 670 (1961); Phys. Rev. 133, A1344 (1964).

[3]See, for example, E. H. Lieb and F. Y. Wu, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. I, pp. 332–487.