# GROUND STATE OF AN ISING FACE-CENTERED CUBIC LATTICE

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Many antiferromagnetic compounds have a face-centered cubic (fcc) magnetic structure. Although in the case of nearest neighbor interactions the ground state of such systems is clearly degenerate, no exact information has been available regarding either the magnitude of its degeneracy or any of its thermodynamic properties. In the case of an antiferromagnetic Ising triangular lattice, it has been shown that the entropy per spin is finite[1] and the zero-field susceptibility infinite[2] at $T=0°$K. In this Letter we show that, assuming nearest neighbor Ising interactions, simple topological and energy arguments lead to a complete classification of the ground-state configurations. Hence, a precise enumeration of the states is possible and exact thermodynamic results are deduced at $T=0°$K.

We consider an antiferromagnetic system consisting of $N$ spin moments on an fcc lattice. Each spin is capable of existing in one of two possible states denoted +, -, and interacts with its nearest neighbors (n.n.) only. The interaction energy is $+J$ for a pair of like spins (++ or --) and $-J$ for a pair of unlike spins (+- or -+).

First, the energy of the ground state of the system is determined. An fcc lattice of $N$ sites can be subdivided into $N$ tetrahedra, such that each n.n. interaction bond is found on one and only one tetrahedron; hence there are a total of $6N$ such bonds. In the ground state, each one of these tetrahedra must be in its own ground state, i.e., two of its spins in the state + and two in the state -. This ground state of the tetrahedron is denoted by the symbol $\omega$, and the corresponding energy is $-2J$. Hence the energy of the ground state of the fcc system is $-2NJ$. It then also follows that every tetrahedron in the lattice is in state $\omega$.

We next consider the fcc lattice built up of layers of triangular lattices. In Fig. 1 such a layer (1) is shown—the circles at the centers of the triangles denote sites on layer (2) which is immediately under layer (1), and points at the centers of the remaining triangles denote sites on layer (3) which is immediately above layer (1). Each triangle of (1) is the base of a tetrahedron, the vertex of which is a site either on (2) or (3). Also, each site on a given layer is the vertex of a tetrahedron, the base of which is a triangle on an adjacent layer.

Since in the ground state of the fcc system each tetrahedron is in the state $\omega$, it follows that each triangle of spins in a given layer should be in one of the states (++-) or (--+). Therefore any triangular layer should also be in one of its ground states. The number of such states is of the order $2^{0.47n}$, where $n$ is the number of spins (or sites) on a triangular lattice.[1]

Thirdly, we note that if the configuration of the ground state of layer (1) is determined, then the configurations of both layers (2) and (3) are also determined. This obtains because each triangle has one of the configurations (++-) or (--+), and since it is also required that each tetrahedron be in the state $\omega$, the state of the spin at the vertex of the tetrahedron is determined, and this vertex is in the adjacent layer. It follows that the ground configurational state of the whole fcc system is determined by the ground configurational state of any one of its triangular layers; hence we can deduce that its degeneracy is $\leqslant 2^{0.47n}$, $n \sim N^{2/3}$. We now proceed to show that the strict inequality holds.

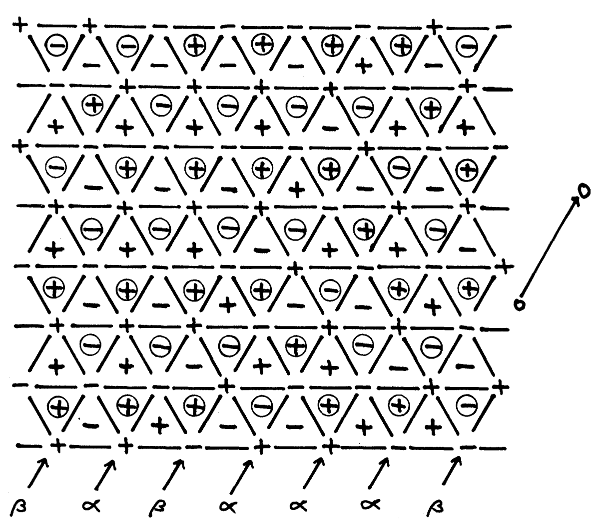

FIG. 1. Three successive layers of a face-centered cubic lattice: layer (1) denoted by triangles; sites on layer (2) denoted by circles; and sites on layer (3) are at the centers of the remaining triangles.

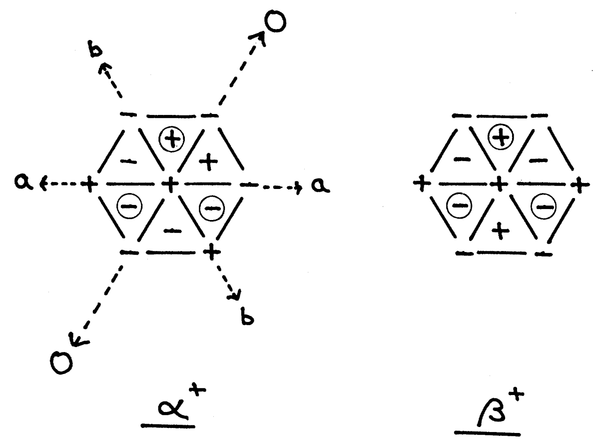


FIG. 2. The $\alpha^+$ and $\beta^+$ clusters. Notation as for Fig. 1.

Figure 2 shows two clusters, each having a central spin with its 12 nearest neighbors. Such clusters contain 8 tetrahedra: 6 having the triangles of (1) as bases, the remaining two having the central spin for their vertices and their bases on layers (2) and (3), respectively. The condition that each tetrahedron must be in the state $\omega$ reduces the number of basic types of such clusters to four. Two of them, $\alpha^+$ and $\beta^+$, are shown in Fig. 2; the other two, $\alpha^-$ and $\beta^-$, are obtained simply by reversing all the spins.

It follows that in the ground state, each + spin is at the center of an $\alpha^+$ or $\beta^+$ cluster and each - spin is at the center of an $\alpha^-$ or $\beta^-$ cluster. The possible ground states of a triangular layer can therefore be obtained by grouping these four clusters. The number of possibilities is restricted by a property of the $\alpha$ cluster. If a particular site—chosen as origin—is the center of an $\alpha$ cluster, then the adjacent clusters along the 00 axis must also be $\alpha$ clusters. Hence all clusters along the 00 axis must be $\alpha$ clusters. On the other hand, adjacent clusters along $aa$ or $bb$ axes may be either $\alpha$ or $\beta$. If one therefore looks at the triangular layer along the 00 direction, one can have a row (parallel to 00) of $\alpha$ clusters followed by another row of either $\alpha$ clusters or $\beta$ clusters. Thus the triangular layer will consist of rows, each consisting entirely of $\alpha$ or $\beta$ clusters (e.g., Fig. 1). The number of arrangements is clearly $2^R$, where $R$ is the number of rows.

The degeneracy of the ground state of the fcc system is therefore $\exp(AN^{1/3}\ln 2)$, and it follows that in the limit $N=\infty$ the entropy per spin tends to zero as $T\to 0°$K.

In the above scheme all triangular layers have identical configurations and since all possible configurations have zero moment, it follows that the susceptibility is zero at $T=0°$K.

I am grateful to Dr. M. F. Sykes for drawing my attention to this problem and for valuable discussions.

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

[2]M. F. Sykes (to be published), based on the theory developed by M. E. Fisher, Phys. Rev. 113, 969 (1959).

## SUPERCONDUCTIVITY AT HIGH MAGNETIC FIELDS AND CURRENT DENSITIES IN SOME Nb-Zr ALLOYS*

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Zero electrical resistance at unusually high magnetic fields and current densities has recently been reported in the compound $Nb_3Sn$,[1,2] and in the alloy Mo−25 at.% (atomic percent) Re.[3] The present results on Nb-Zr alloys were obtained during the course of a systematic investigation of resistive superconducting transitions in certain Ti, Zr, Nb, Hf, and Ta-rich binary alloys in magnetic fields up to 30 kgauss. The data show that cold-worked Nb-rich Nb-Zr alloys display zero electrical resistance at current densities as high as $10^5$ amp/cm$^2$ at 30 kgauss and at 4.2°K.[4,5] As far as we are aware, only the specially prepared Nb-clad "$Nb_3Sn$" cores of Kunzler et al.[1] have exhibited greater zero-resistance current-carrying capacities above 10 kgauss. The present measurements also reveal some interesting high-field superconducting effects in cold-rolled Nb-Zr alloys: (a) a marked dependence of the magnitude of