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ANTIFERROMAGNETIC ORDERING IN AN ISING LATTICE BY A MONTE CARLO METHOD

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The magnetic properties of face-centered cubic antiferromagnetic crystals do not agree well with simple molecular field theory, and a spin-wave approach is only reliable at very low temperatures. For this reason an attempt to understand the apparently anomalous magnetic properties[1] of MnO in the region of the transition temperature has been made by an extension of the molecular field approach using a Monte Carlo method. This method of treating problems in statistical mechanics, which is made feasible only by the use of a high-speed computer, was first used by Metropolis and others[2] and has been applied to ordering in crystal lattices by Ehrman, Fosdick, and Handscomb[3] and by Handscomb.[4]

In the simplest molecular field approximation, the exchange interactions between a spin and its neighbors are replaced by an effective field which is proportional to the sublattice magnetization. MnO has type-II order so that any spin has its 6 next nearest neighbors (n.n.n.) all antiparallel, but of its 12 nearest neighbors (n.n.) 6 are parallel and 6 antiparallel. This means that the n.n. do not contribute to the effective field, which is given by

$$g\beta H_E = 6J_2\langle S_z\rangle,$$

where the n.n.n. interaction is of the form $J_2\vec{s}_i\cdot\vec{s}_j$. So in this approximation, the magnetic properties should be independent of the n.n. interaction. In reality, as the temperature rises from zero, n.n. interactions must lead to short-range n.n. ordering, and this increases with temperature, eventually destroying the long-range order at a lower temperature than that predicted by the simple theory. The present method allows for this.

The calculation proceeds as follows:

(1) Each spin in a block of 384 spins forming a fcc lattice is represented by a variable in the computer. Continuity at the boundaries of the block is obtained by linking the top to the bottom, the left-hand side to the right-hand side, and so on. Each of these variables can take one of the $2S+1$ values, $M_i = -S, -S+1, \cdots, +S$, and the configuration at any moment is specified by these 384 numbers.

(2) Some initial configuration is set up, either ordered or disordered.

(3) Each site is now considered in turn. (a) The effective field at site i is computed in terms of the magnetic quantum numbers of its 12 n.n. (M_j) and 6 n.n.n. (M_k):

$$g\beta H_E = J_1\textstyle\sum_j M_j + J_2\sum_k M_k.$$

(b) The energies of the possible states for M_i are computed:

$$E_i = g\beta H_E M_i.$$

(c) A new value for M_i is selected by a pseudo-random process such that the probability of selecting any particular value is proportional to

$$P = e^{-E_i/kT}.$$

It is this new value which is used when treating subsequent sites. When all 384 sites have been considered, the whole cycle is repeated.

(4) At the end of each cycle, information is extracted about the state of magnetic ordering. In order to allow for different types of order, the lattice is divided into 32 sublattices, so that no spin lies on the same sublattice as any of its n.n. or n.n.n. The magnetization $\langle M_i\rangle$ is computed for each sublattice. A long-range ordering parameter is defined as the average of the moduli of these. Short-range ordering is measured

by $\langle M_i M_j \rangle$ averaged over all n.n. pairs, and by $\langle M_i M_k \rangle$ averaged over all n.n.n. pairs.

(5) The calculations are terminated when the parameters cease to show any regular variation, but just a random scatter about a mean value which is independent of the initial configuration.

Figure 1 shows the results of computations using spins $S = \frac{5}{2}$, with various values for T and J_1/J_2. T_N is taken to be that temperature at which the sublattice magnetization is changing most rapidly, and this is drawn so as to drop to zero at this temperature. By inspection it is found that above this temperature the individual sublattice magnetizations often change sign from one cycle to the next. Because of the boundary conditions, successive cycles can be regarded as describing adjacent blocks of spins in an infinite lattice, so this change of sign indicates a breakdown of the long-range order. The long-range ordering parameter as defined above is

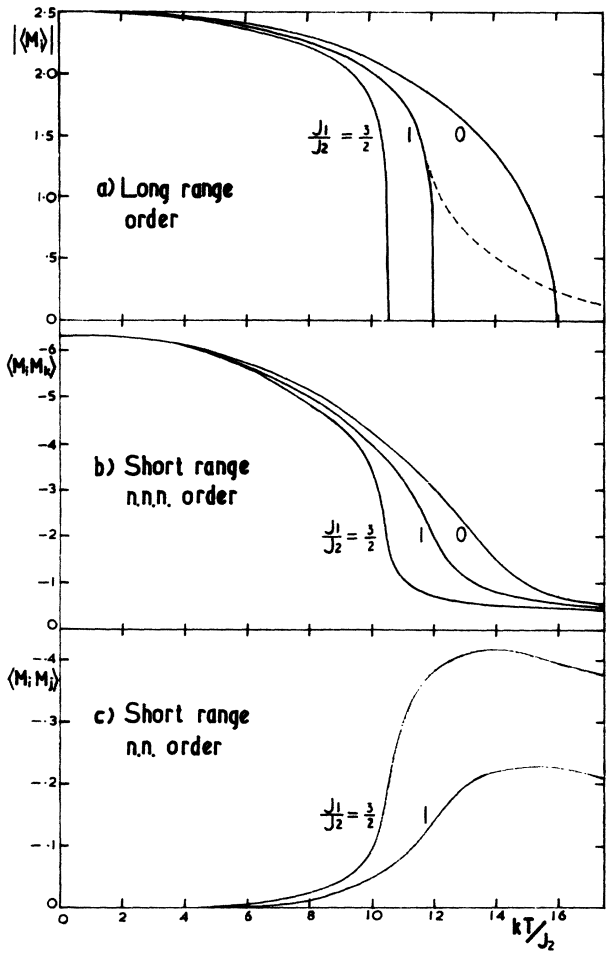

FIG. 1. Computed ordering parameters as a function of kT/J_2 and J_1/J_2.

then no longer relevant to an infinite lattice, but only to a region the size of our small lattice. If plotted out it gives a tail to the sublattice magnetization curve [shown dashed in Fig. 1(a) for $J_1/J_2 = 1$], and this tail can be expected to depend on the size of the lattice being considered. It is interesting to note that a similar tail was obtained in measurements on neutron scattering in MnO by Shull, Strauser, and Wollan[5] and they also attributed this to medium-range ordering.

One effect of J_1 is to make the transition temperature lower than that predicted by simple molecular field theory, and more in agreement with the spin-wave results of Ziman.[6] For $J_1 = J_2$, the present work indicates $T_N = 12J_2/k$, compared with molecular field $T_N = 17.5J_2/k$, and Ziman's result, $T_N = 9J_2/k$.

Pair measurements[7] on Mn in MgO suggests that $J_1/J_2 = 1$. The shape of the sublattice magnetization curve computed with this value is compared with results from neutron-scattering measurements on MnO in Fig. 2. The magnetization is given by (neutron intensity)$^{1/2}$, and the shape of the curve is in good agreement with other experimental measurements.[1] The present results are seen to be an improvement on the Brillouin curve calculated by molecular field theory. It may be pointed out, however, that the Brillouin curve can be modified to give better agreement by allowing for thermal expansion,[8] a small effect in MnO, or by introducing a small biquadratic exchange interaction.[9]

The interpretation of the present computations

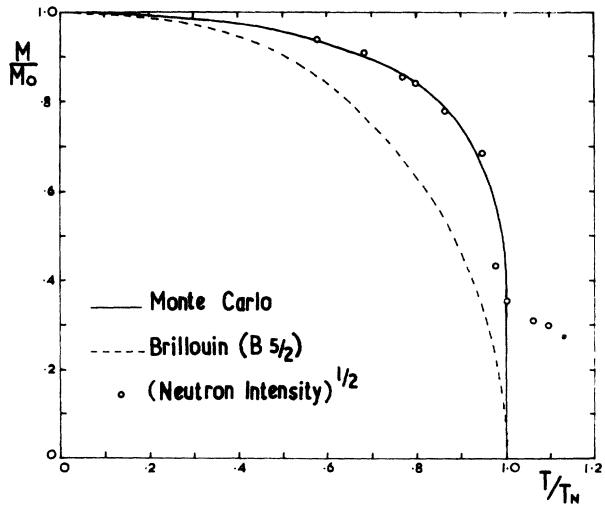

FIG. 2. The temperature variation of the sublattice magnetization of MnO. Experimental points, measured by Shull, Strauser, and Wollan (reference 5) are compared with the computed curve where $J_1/J_2 = 1$.

is limited by the small lattice of spins considered, and a larger lattice would almost certainly give slightly different results. However, the method certainly provides useful results, and indicates the power of a Monte Carlo approach to this type of problem.

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INFLUENCE OF THE PHONON SPECTRUM ON THE DENSITY OF ELECTRON STATES IN SUPERCONDUCTING TANTALUM

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A tunnelling experiment has been performed on superconducting tantalum which suggests that electron-phonon interactions are responsible for the superconductivity in Ta, as they are in nontransition-group metals. This conclusion results from the observation of the influence of the phonon spectrum on the density of states of Ta; this is the first report of such an influence in a transition metal.

Superconducting metals can be divided into two groups, transition and nontransition metals. The critical temperatures of the superconductors in the transition group have a periodic dependence on their number of valence electrons. This is Matthias's rule.[1] Nontransition elements do not obey such a rule and this difference among others has led to the suggestion[2] that perhaps the mechanisms for the superconductivity in the two groups are different.

The success of the electron-phonon interaction in nontransition-group superconductors is epitomized by the detailed agreement of the tunnelling experiments on Pb by Rowell, Anderson, and Thomas[3] and the theoretical calculations of Schrieffer, Scalapino, and Wilkins,[4] and Scalapino and Anderson.[5] The current-voltage (I-V) characteristic of the Pb tunnel junctions showed structure which could be classified into two groups, the relatively large structure which is due to the peaks in the phonon spectrum $g(\nu)$ vs ν and the smaller structure which is associated with the Van Hove and other critical points in $g(\nu)$ vs ν. The density of states and hence the I-V characteristic reflect the sum of both these effects.

We have made similar tunnelling measurements on Ta to measure the effect of its phonon spectrum.

The tunnel junctions were made on bulk specimens of Ta because these can be made much more pure than films. Best commercial quality Ta was rolled into a foil 0.003 in. thick, and from this were cut pieces 1 in. long and 0.1 in. wide. After a chemical etch, the specimens were outgassed by heating to their melting points over many hours in a vacuum of $\lesssim 10^{-8}$ mm. The surface of the foil was then coated with GE varnish 7031 leaving clear a strip ~0.01 in. wide along the length of the specimen. This strip was then oxidized at 50°C in oxygen for a few hours and then cross strips of Ag were evaporated on. The junctions had a resistance of ~200 Ω and an area of $\sim 10^{-3}$ cm^2.

At helium temperatures the junctions showed the usual I-V characteristic for a normal superconductor-insulator-metal tunnel junction. At the lowest temperature, 0.9°K, the first derivative (dV/dI) and the second derivative (d^2I/dV^2) of the I-V characteristic were measured as a function of dc bias. dV/dI was measured by applying a constant small ac current (0.5 μA) through the sample and measuring the ac voltage