Nearest-neighbor Ising antiferromagnet in a magnetic field—the body-centered-cubic lattice*

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The results of a Monte Carlo study of a nearest-neighbor Ising antiferromagnet in an external magnetic field are reported. The effect of the presence of the field on the order-disorder transition is discussed, and the alternating long-range order, staggered susceptibility, ordinary susceptibility, and specific heat as functions of temperature for several fields are presented. For small fields, the calculation is consistent with the results of series expansions, but near the critical field it disagrees with the series extrapolations, and supports qualitatively the prediction of molecular-field approximations, namely, that there can be two transitions provided that the field is slightly larger than the $T = 0$ critical value.

INTRODUCTION

The purpose of this paper is to report the results of a Monte Carlo study of the body-centered-cubic (bcc) Ising antiferromagnet in the presence of an external magnetic field. The calculations were carried out on lattices of 8192 and 31 250 sites with periodic boundary conditions. We present graphs displaying the temperature dependence of long-range order for $N = 31\,250$ sites and staggered susceptibility, ordinary susceptibility, and specific heat for $N = 8192$ sites, at magnetic fields below, equal to, and slightly above the $T = 0$ critical value, B_c. This paper contains a more detailed account of results previously reported.[1]

Since the use of Monte Carlo techniques to study the thermodynamic behavior of Ising systems has been described in recent reviews,[2,3] a detailed mathematical discussion of the techniques will not be given here. However, we emphasize that we have followed the procedure used by Yang[4-6] which differs from the method implemented by most other workers. Each run involved up to 1800 Monte Carlo steps per spin (cycle) for the lattice of 8192 sites, while only 250 cycles were used for the much larger lattice. The initial lattice configuration was usually the zero-field ground state but selected points were also computed using a disordered initial state as a check. A subjective judgement was made as to how many cycles were sufficient to remove the effect of the initial state by examining the cycle-by-cycle behavior of long- and short-range order. Usually 100 cycles were deleted from the ensemble data. The relatively small number of cycles used here precluded a quantitative study of behavior extremely close to $T_c(B)$. The qualitative evidence for the existence of the phase transitions is, therefore, to be emphasized.

The calculations were based on the Hamiltonian

$$H = J \sum_{ij} \delta_i \delta_j - mB \sum_i \delta_i , \quad J > 0, \; B \geq 0 , \tag{1}$$

where J is the exchange integral, m is the magnetic moment per spin, B is the strength of the external field, the double summation is over nearest-neighbor pairs, and $\delta_i = \pm 1$.

The equilibrium thermodynamic value of any quantity x is given by

$$\langle x \rangle = \sum x e^{-\beta H} \Big/ \sum e^{-\beta H}, \tag{2}$$

with the summation taken over all accessible states and $\beta = 1/kT$. The Monte Carlo method provides an approximation to the ensemble average (2).

The bcc lattice can be decomposed into two interpenetrating sublattices such that each site has nearest neighbors only on the other sublattice. Let N_{1-} and N_{2-} be the number of down spins on sublattice 1 and 2, respectively. It is convenient to define an alternating long-range order parameter S as

$$S = \langle (N_{1-} - N_{2-})/(N_{1-} + N_{2-}) \rangle \quad . \tag{3}$$

In computing S we define the ratio inside the brackets to be zero when all spins are up (parallel to B).

In the absence of a field, $|S| \to 1$ as $T \to 0$, and $S = 0$ at $T = \infty$. Furthermore, S is identical with the magnetization of the Ising ferromagnet due to the well-known one-to-one correspondence of states of the two models. Hence, the appearance of long-range order S signifies a second-order transition in the antiferromagnet. Associated with the ferromagnetic transition there is a singularity in the magnetic susceptibility χ. Series expansions[7] indicate that χ is finite for the bcc antiferromagnet in zero field. The staggered susceptibility χ_s for the antiferromagnet is identical to the ferromagnetic susceptibility in zero field and is, therefore, singular at the transition. The specific heat C is also singular in zero field. In terms of ensemble averages, these quantities are for a finite lattice of N sites,

$$kT\chi_s/4Nm^2 = [\langle (N_{1-} - N_{2-})^2\rangle - \langle N_{1-} - N_{2-}\rangle^2]/N\ , \qquad (4)$$

$$kT\chi/4Nm^2 = (\langle N_-^2\rangle - \langle N_-\rangle^2)/N,\quad N_- = N_{1-} + N_{2-}\ , \qquad (5)$$

$$C/k = \beta^2[\langle H^2\rangle - \langle H\rangle^2]/N\ . \qquad (6)$$

The introduction of an external field destroys the ferromagnetic transition but not the antiferromagnetic one. Long-range order should still appear, but at a lower temperature, and this should be accompanied by a strong singularity in the staggered susceptibility.[8] $|S| \to 1$ as $T \to 0$ is certain, however, only if the external field has a magnitude less than the critical value $B_c = \gamma J/m$, where γ is the coordination number of the lattice ($\gamma = 8$ for bcc). For $B > B_c$, the ground state has all spins parallel to the field. For $B > B_c$ and at sufficiently low temperatures the number of minority spins (down spins) will be small enough that they will be evenly distributed between sublattices ($|S| = 0$).

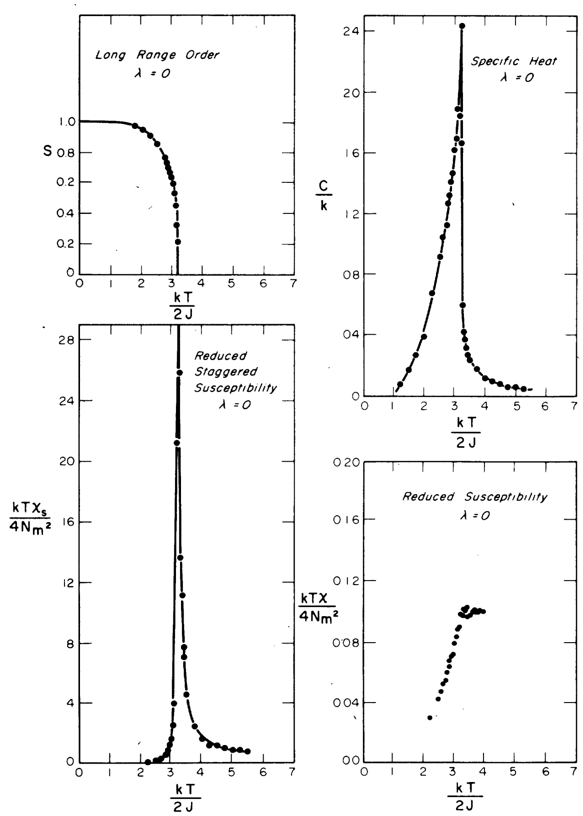

FIG. 1. Zero-field behavior of the bcc nearest-neighbor Ising antiferromagnet. The data points are Monte Carlo results. The long-range order and reduced staggered susceptibility are plotted along with Padé approximants (solid curves) from Refs. 13 and 14. A curve is freely drawn through the specific-heat data.

Thus it is natural to presume that no transition occurs at any temperature when $B > B_c$.

Previously, molecular field approximations,[9-11] as well as series expansions,[12] have been applied to this model. All of these approximations show the depression of the critical temperature T_c with increasing B. They disagree quantitatively. Furthermore, the molecular field calculations disagree qualitatively with the series expansion study of Bienenstock[12] on the question of the presence of a transition for fields equal to and greater than B_c. The former studies[9-11] predict the existence of a transition for $B = B_c$ and two transitions for $B \gtrsim B_c$, while the latter[12] provides no evidence for this phenomenon. Padé approximant extrapolations[13,14] of series expansions have provided what are believed to be extremely accurate quantitative results for the zero-field transition, and one hopes for similar success in other cases. Molecular field approximations are known to be quantitatively wrong in the zero-field case, and Ziman[10] conjectured that the exact solution to the bcc Ising antiferromagnet would not have the feature of two transitions. This opinion was supported by Fisher's exact solution[15] of the two-dimensional super exchange antiferromagnet. Thus there is a tendency to believe that the series expansion result is closer to the truth. The Monte Carlo method provides an independent approach to this problem and the study described in this paper indicates that Ziman's conjecture is incorrect.

RESULTS

We present in Fig. 1 the long-range order, staggered susceptibility, specific heat, and susceptibility as functions of temperature for zero field. The long-range order and staggered susceptibility are compared with the Pade approximants.[13,14] As can be seen, there is excellent qualitative agreement for both quantities and quantitative agreement away from T_c. We hope for similar accuracy when applying the method to the case of an external field.

In Fig. 2, we present several of the alternating long-range order curves in the presence of an external field B. The depression of the critical temperature with increasing B is evident. The transition temperature does not approach 0 as $B \to B_c$, however. The lattice clearly orders at finite temperature in the critical field, although total order is never attained. Just above the critical field, the lattice still orders, the long-range order parameter reaching a maximum value less than 1.0 as temperature is lowered, and then the order parameter decreases to zero at a still lower but finite T. Thus there appear to be two transitions in

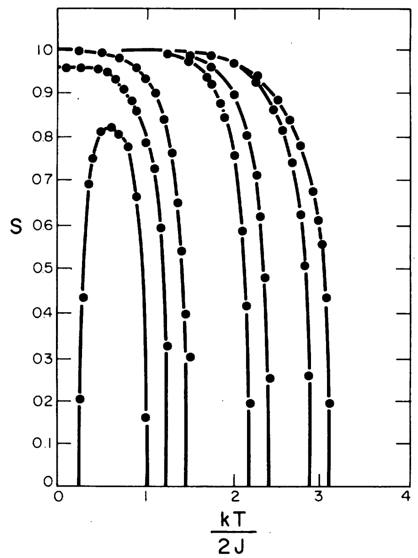

FIG. 2. Long-range order vs reduced temperature for several fields. Right to left, λ=2, 4, 6, 6.7, 7.8, 8.0, 8.1.

fields slightly larger than B_c. The two transitions remain for even higher fields, but the critical temperatures become closer together until they merge and the transitions disappear altogether. As we pointed out in a previous note,[1] the behavior of long range order is qualitatively the same as that predicted by the Bethe-Peierls[10] approximation, and also supports the prediction of the mean field[9] and Kikuchi[11] approximations that the model does

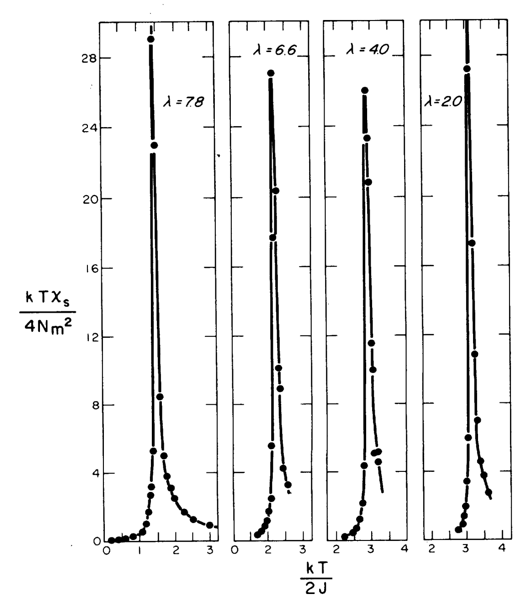

FIG. 3. Reduced staggered susceptibility vs reduced temperature for several fields.

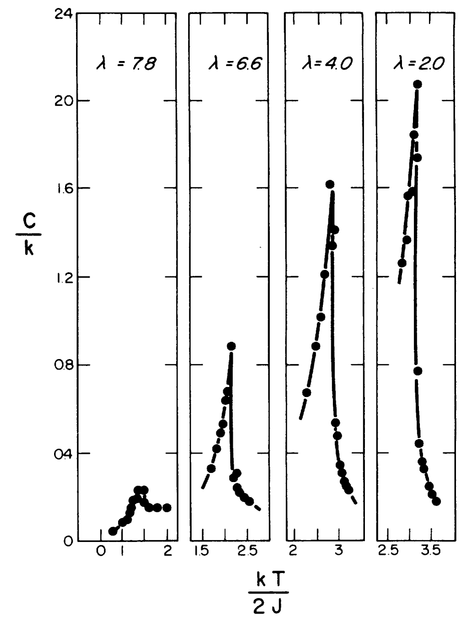

FIG. 4. Specific heat vs reduced temperature for several fields.

contain the feature of two transitions.

Even in the presence of an external field, the staggered susceptibility is expected[8] to exhibit a strong singularity at T_c. In Fig. 3, we present four staggered susceptibility curves for a lattice of 8192 sites in external fields. The peak remains strong for each $\lambda = mB/J$, and each curve indicates a transition temperature that agrees with that indicated by the corresponding long-range-order curve.

In Fig. 4, we show the corresponding specific heat for each λ. The height of the peak is clearly

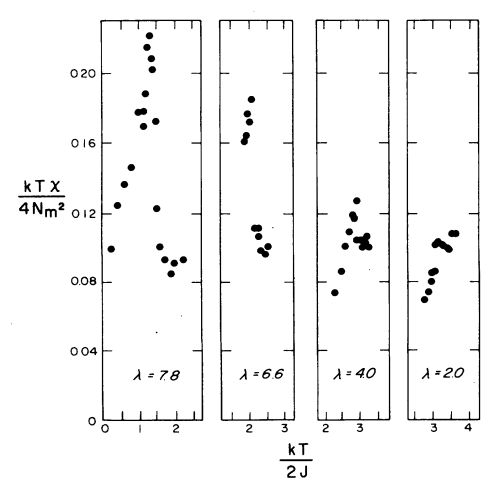

FIG. 5. Reduced susceptibility vs reduced temperature for several fields.

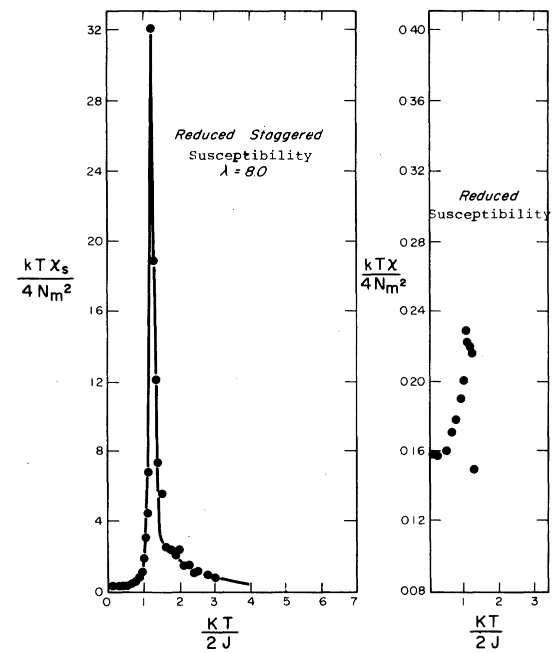

FIG. 6. Reduced staggered susceptibility and reduced ordinary susceptibility in the critical magnetic field.

diminished by the presence of the field so that the specific heat anomaly becomes less pronounced with increasing B. This behavior resembles that of the two-dimensional super exchange antiferromagnet of Fisher.[15] Although they are of less quality, the susceptibility curves shown in Fig. 5 also resemble in some respects the susceptibility of the super exchange antiferromagnet. There is no sharp peak in zero field, but as the field is increased, a peak seems to appear and grow with B.

In Fig. 6, we show the staggered susceptibility and ordinary susceptibility in the critical magnetic field $\lambda = \lambda_c = 8.0$. The strong peak in the staggered susceptibility provides striking evidence of a phase transition in this field. The ordinary susceptibility also exhibits an anomaly.

Finally, in Fig. 7, we present the staggered susceptibility for $\lambda = 8.1$ which is slightly larger than the critical value. The two peaks observed are evidence of two separate transitions associated with the appearance and then disappearance of alternating long range order. We made computations at $\lambda = 8.2$, and found that long-range order did seem to appear and then disappear as temperature was varied and the corresponding staggered susceptibility definitely had large values in the same temperature region but the closeness of the two transitions made it impossible to distinguish two separate peaks and also caused the long-range order curve to be of poor quality.[1] At $\lambda = 8.3$, our results indicated that the transitions had completely disappeared.

The microscopic structure of the phases for $\lambda = 8.1$ was examined by printing out the lattice configuration after the last cycle of computation. For large T, there was an apparent random distribution of minority spins throughout the lattice. At intermediate temperatures near the long-range order maximum, the configurations showed the tendency for minority spins to accumulate on one of the sublattices, the state resembling those found for low temperatures and small fields. At temperatures between zero and the low-T transition a state of high short-range order was observed. However, the minority sites were evenly distributed between the sublattices.

DISCUSSION

Our results indicate that the critical temperature decreases with increasing field, but does not approach zero at the critical value. Instead, there is a transition at finite T for $B = B_c$. In a small range of fields above B_c, there are two transitions corresponding to the appearance and then disappearance of alternating long-range order as tem-

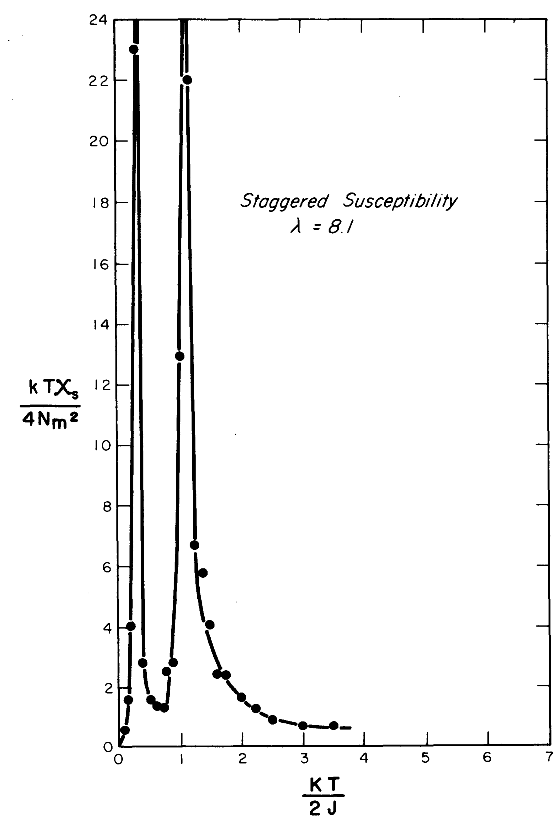

FIG. 7. Reduced staggered susceptibility vs reduced temperature in a field slightly greater than the critical value.

perature is lowered. Each transition is accompanied by a peak in the staggered susceptibility, suggesting a singularity in this function for an infinite lattice similar to that found in zero field. Although our data agrees with series data for small fields it is in substantial disagreement near the critical field with the series expansion study of Bienenstock.[12] From the staggered susceptibility at $\lambda = 7.8$, we can estimate the critical temperature to within, at worst, 10%. We take as our estimate $T_c(7.8)/T_c(0) = 0.46$, whereas Bienenstock obtains 0.34, a discrepancy of 26%. The transition in the critical field, the two transitions above B_c, and the tendency for the transitions to become closer together as B increases beyond B_c implies that the critical curve (B vs T_c) for the bcc antiferromagnet must exhibit a slight "bulge" similar to that shown in Fig. 2 of Ref. 1. The bulge is smaller than that predicted by the Bethe-Peierls[10] study, since our calculation indicates that the transitions disappear at a smaller field.

It is plausible that the model could exhibit this two transition phenomenon. The antiferromagnetic interaction tends to anti-align spins and hence to produce short-range and ultimately long-range alternating order. Thermal activity tends to destroy this order. The ordinary transition consists of the overcoming of thermal effects by the spin-spin interaction such that alternating long-range order extends throughout the lattice. As temperature is lowered, the relative importance of the spin-spin interaction is increased so that long-range order becomes total at $T = 0$. With the introduction of an external magnetic field B, the situation becomes more complicated. The field tends to align spins with itself and hence with one another, which opposes alternating order. As a result, the transition temperature must be lower in the presence of B.

Clearly, for $B > B_c$, $S \to 0$ as $T \to 0$. It is, however, possible although not obvious that long-range order might appear at finite T for $B \gtrsim B_c$. If the average number of downspins is large enough, then states with alternating order will be preferred (for a given number of downspins) over states with less alternating order (for the same number of downspins) since the former states will have a lower energy than the latter states. In other words, since the relative fluctuation in the number of downspins (minority spins) is small away from a transition, the lattice can be viewed as having a fixed number of minority spins at particular values of B and T. If this number of minority spins is large enough then states with more minority spins on a particular sublattice will be preferred and hence the average long-range alternating order may be nonzero. As the temperature is lowered, the average number of minority spins will decrease until it is small enough that the minority spins can easily move between sublattices while rarely becoming nearest neighbors. In this case the minority spins will be evenly distributed between the two sublattices and so the average long-range order will be zero. Thus for $B \gtrsim B_c$ we expect $S = 0$ for $T \approx 0$ and also for $T \gg 0$. If $S \neq 0$ for intermediate temperatures we expect two transitions as T is varied for fixed B.

A special case is that of behavior in the critical field itself. For $B = B_c$, the ground state is highly degenerate, and among the many states of lowest energy there are those with long-range order parameters equal to zero, those with long-range order equal to unity, and many values in between. The equilibrium value of S is an average over all accessible states at $T = 0$. Our results show that S approaches a limiting value between zero and one as $T \to 0$ at B_c. This effect is similar to the limiting behavior of the magnetization in Fisher's superexchange antiferromagnet,[15] which does not approach zero as $T \to 0$ in the critical field.

The behavior of the specific heat and susceptibility resemble that of the two-dimensional superexchange antiferromagnet.[15] Fisher's model has a specific heat which remained singular in the presence of an external field; however, the amplitude of the singularity decreased with field. The susceptibility became infinite only in nonzero field, the amplitude of the singular part increasing with the field. The small amplitude of this singularity may explain the relatively poor quality of our susceptibility data, since a weak anomaly can thus be expected to exist in the finite lattice susceptibility. Fisher conjectured that the three-dimensional models would exhibit this kind of behavior. Our results overall are consistent with this except for the two-transition phenomenon.

The differences in lattice structure between the bcc and square lattices may explain the differences in thermodynamic behavior indicated here and that of Fisher's model.

CONCLUSION

We have presented results of a Monte Carlo study of the bcc nearest-neighbor Ising antiferromagnet in an external magnetic field. Our results indicate that the critical temperature is depressed as the field increases, and approaches a finite value as $B \to B_c$. Above and close to B_c, there are two transitions in qualitative agreement with the Bethe-Peierls approximation.[10] Our results disagree with the series expansion study of Bienenstock[12] near the critical field, indicating that the expansion was too short to provide correct results for low temperatures and strong fields. Our results further indicate that below the critical field the three-dimensional antiferromagnet will behave in a way similar to the two-dimensional superexchange model.

It is hoped that this work will lead to extensive simulations which can reveal more quantitatively the critical behavior of Ising antiferromagnets near the critical field.[16]

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