Monte Carlo study of the critical temperature of a two-dimensional, ferromagnetic, binary, Ising system

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A Monte Carlo simulation was used to determine the critical temperature of a two-dimensional, ferromagnetic, binary, quenched Ising alloy as a function of the relative species concentration and of the relative interaction energy between unlike ions. Considering the system to be composed of two ionic species, A and B, we used different B-ion concentrations of 0.25, 0.50, and 0.75. For each of these, the four different values of the relative A-B interaction energy studied were $J_{AB}/J_{AA}=0$, 1, 2, and 4. The value of J_{BB}/J_{AA} was set equal to 4 for all cases. Improvements over the results obtained from mean-field theory, the Bethe-Peierls approximation, and the "effective-field" model of Honmura *et al.* are discussed.

Over the last several years the theory of phase transitions in ferromagnetic, binary, Ising systems has received considerable attention from both a bond and a site perspective.[1-6] The bond model considers all lattice sites to be equivalent, but the interaction energy between each pair of adjacent sites is randomly assigned one of a set of possible values. In the site model, however, the lattice sites are randomly occupied by two different species of magnetic ions, A and B, and the interaction between two ions is determined entirely by the species of those ions. The Hamiltonian for the system is then

$$\mathscr{H}=-\sum_{\langle ij\rangle}[J_{AA}\delta_{iA}\delta_{jA}+J_{BB}\delta_{iB}\delta_{jB}+J_{AB}(\delta_{iA}\delta_{jB}+\delta_{iB}\delta_{jA})]S_iS_j\ ,$$

where the J_{ij}'s are the interaction energies between type-i and type-j ions, the S's are the spin variables ($=\pm1$), and the sum is over all nearest-neighbor pairs.

The site problem has been solved exactly in one dimension,[1] but for higher-dimensional systems various approximations had to be used. In particular, mean-field theory,[2,3] and the Bethe-Peierls approximation[4] have been used to obtain solutions. More recently, a new "effective-field" model[5] has been developed and applied to the site problem. In addition, combinations of approaches have been tried, e.g., a three-dimensional, binary, magnetic system has been modeled by considering it as a set of one-dimensional chains coupled by a mean field.[7] But, as it is well known from the classical monatomic Ising system, these approximations should be expected to yield results that are significantly different from those obtained from an exact solution.[8]

Although the binary magnetic site problem has not been solved exactly, the method of Monte Carlo simulation can be expected to provide results that would be very close to any such solution.[9] The only previous Monte Carlo work done on the site problem has been that of Tatsumi.[6] His work, however, had different objectives from that presented here. Tatsumi considered spin-glass transitions in a binary system arrayed on a simple-cubic lattice. In order to examine the spin-glass state, an antiferromagnetic interaction must be present. In this work we deal only with ferromagnetic interactions on a square lattice and seek to establish the best estimates yet made for the critical temperatures in the two-dimensional, binary, magnetic site model.

The critical temperature of a ferromagnetic, binary alloy was determined for three values of nominal B-ion concentration, 0.25, 0.50, and 0.75. These results, together with those for the pure lattice cases of $p_B=0.0$ and 1.0, were sufficient to establish the behavior of the critical temperature as a function of concentration. For each of these p_B values, four different values of J_{AB}/J_{AA} ($=0$, 1, 2, 4) were studied. This particular selection was made due to the choice of $J_{BB}/J_{AA}=4$, and arbitrary value, but one that provided a convenient temperature range in which to work.

All systems studied consisted of random arrangements of A and B ions on a 40×40 square lattice with periodic boundary conditions. The ion types, A and B, were assigned randomly, simulating a quenched system. The Monte Carlo (MC) procedure first developed by Metropolis *et al.*[10] was used to generate, for a fixed value of k_BT/J_{AA}, successive microstates of the system from which statistical data on the order parameter and energy were generated.

The order parameter for the ferromagnetic binary alloy was defined to be the absolute value of the magnetization:

$$|M|=\left|\sum_i S_i\right|/N^2\ ,$$

where N is the length of a side of the lattice.

The absolute value was used since, without an external field, there was no preferred spin direction, and the ordered state could appear with the majority of spins pointing down, as well as up. Values of the order parameter and energy of the system were recorded after each lattice pass, and the final state of the system was used as the initial state for the next pass. The procedure continued for 3500 passes. Before computing average values of the order parameter and energy for the entire set, the results for

the first 500 passes were discarded so as to minimize any effects due to the original spin configuration (all spins up). In order to compile better statistics, three independent sets of data were collected. Therefore, the results for each reduced temperature were based on a total of 9000 passes.

Another reason for using three independent sets was to be able to take better account of the correlation effects known to be present in each set of 3000 data points, i.e., since the final spin configuration after one lattice pass was used as the initial configuration for the next, the trials were not truly independent. Correlations must be considered in the uncertainty analysis. The simplest way to account for these effects was to use the concept of "statistical inefficiency" (SI) as discussed by Friedberg and Cameron[11] and by Landau[12] for such MC simulations. The SI is the factor by which the variance of the mean (calculated in the usual way assuming no correlations) should be multiplied to obtain a more realistic estimate of the uncertainty. The actual values of the SI obtained from the data depended on the reduced temperature but were about 100 near the critical point for all cases.

The averages and uncertainties of the order parameter and energy for the three individual sets then had to be combined to obtain the appropriate values for all 9000 trials. The overall averages for both quantities were simply the averages of the set averages. The SI value to be associated with the variance of the combined data was taken to be the average of the SI's computed for the three separate sets. Although this was an estimate of the overall SI, it should be entirely adequate for this work.

An attempt was made to find the critical temperature for each case from the peak in the heat capacity as a function of temperature. Ferdinand and Fisher[13] have shown that for a finite, two-dimensional, square Ising system with periodic boundary conditions,

$$(T_c - T_m)/T_c = -0.3603/N \ ,$$

where T_c represents the critical temperature for the infinite system and T_m is the critical temperature for the finite system as determined by the peak in the heat capacity. In the present study, with $N=40$, the expected overestimate of the critical point based on the heat-capacity peak would have been on the order of 1%. However, the heat-capacity peak for our data was too broad to make possible a reliable estimate of the critical temperature.

Therefore, it was decided to use finite-size scaling theory to calculate the reduced critical temperature, $T_{rc}=k_B T_c/J_{AA}$, for the infinite system directly from the $|M|$ data for the finite system. It has been shown[12,14,15] that for a finite, two-dimensional Ising system

$$|M| \propto N^{-\beta/\nu}(\epsilon N^{1/\nu})^{\beta}, \quad T < T_c$$

where

$$\epsilon = \left| \frac{T - T_c}{T_c} \right|$$

and the critical exponents for the two-dimensional lattice are $\beta=\frac{1}{8}$ and $\nu=1$.

To obtain a value of T_{rc} for a particular case, graphs of $|M|N^{1/8}$ versus ϵN were constructed on a log-log scale for a series of estimates of T_{rc}. For each graph the only data used were for reduced temperatures below the estimated T_{rc} and ϵN values between 0.2 and 10. There were always at least seven, often more, points which met these criteria, and, as was the case with Landau's data,[12] the points did show good linearity over this range of ϵN. The uncertainties in $|M|$ were taken into account in the fitting procedure. The best estimate of T_{rc} was taken to be that value for which the slope of the fitted line was closest to $\frac{1}{8}$. The uncertainty in T_{rc} was determined by the range of estimated T_{rc} values whose corresponding slopes plus or minus the slope uncertainties could equal $\frac{1}{8}$.

As can be seen in Table I, the uncertainties in the T_{rc}'s produced by this procedure were very small, probably too small. A few cases were completely rerun with different sets of random numbers. The T_{rc}'s for the new runs were within about 1% of the values shown in Table I, but not always within the calculated uncertainties. Furthermore, it will be noted that the T_{rc} values computed for the pure cases were about 1% above the exact values. It is believed to be coincidental that the Monte Carlo results for T_{rc} exceeded the exact results by approximately the same amount as Ferdinand and Fisher showed the finite-size T_m should exceed T_c. Lastly, it should be remembered that the T_{rc}'s were determined for particular configurations of A and B spins; some variation in T_{rc} would be expected for different configurations. This is suggested by the data for the cases of $p_B=0.25$, $J_{AB}/J_{AA}=4$;

TABLE I. Monte Carlo results for reduced critical temperature, $k_B T_c/J_{AA}$, for different values of B-ion concentration (nominal and actual) and J_{AB}/J_{AA}. The uncertainties listed are those calculated from using finite-size scaling theory to fit the data.

p_B			
Nominal	Actual	$\frac{J_{AB}}{J_{AA}}$	$\frac{k_B T_c}{J_{AA}}$
0.000	0.000		2.29±0.01
0.250	0.265	0	1.35±0.01
	0.263	1	2.54±0.01
	0.239	2	3.26±0.02
	0.253	4	4.74±0.02
	0.260	4	4.84±0.02
0.500	0.520	1	3.92±0.01
	0.494	2	4.83±0.02
	0.497	2	4.90±0.01
	0.494	4	6.86±0.03
0.750	0.751	0	5.60±0.01
	0.744	1	5.82±0.02
	0.751	1	5.99±0.03
	0.740	2	6.90±0.02
	0.751	4	8.63±0.2
1.000	1.000		9.15±0.01

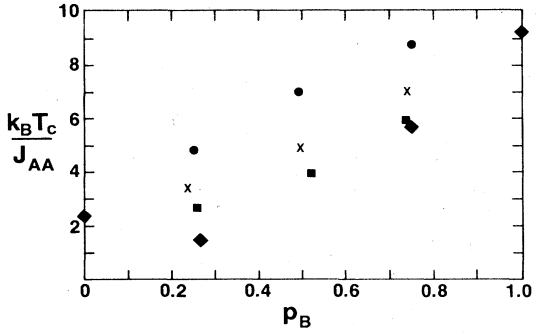

FIG. 1. Monte Carlo simulation results for reduced critical temperature, $k_B T_c/J_{AA}$, as a function of B-ion concentration for different values of J_{AB}/J_{AA}. Key: ◆, $J_{AB}/J_{AA}=0$; ■, $J_{AB}/J_{AA}=1$; ×, $J_{AB}/J_{AA}=2$; ●, $J_{AB}/J_{AA}=4$.

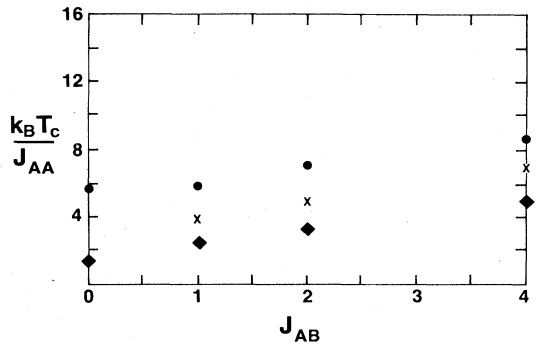

FIG. 2. Monte Carlo simulation results for $k_B T_c/J_{AA}$ as a function of J_{AB}/J_{AA} for different values of nominal B-ion concentration. Key: ◆, $p_B=0.25$; ×, $p_B=0.50$; ●, $p_B=0.75$.

$p_B=0.50$, $J_{AB}/J_{AA}=2$; and $p_B=0.75$, $J_{AB}/J_{AA}=1$. Note, however, that in each case T_{rc} did increase as the actual p_B increased. For all of the above reasons, it is believed that the uncertainties in the T_{rc}'s are actually about 1%.

The results for the critical temperatures as a function of p_B for the different values of J_{AB}/J_{AA} are shown in Fig. 1. For the $J_{AB}/J_{AA}=0$ case, T_{rc} initially drops as p_B increases from 0 and would, on the basis of percolation theory,[16] be expected to fall to zero at $p_B=0.41$. Similarly, as p_B decreases from 1, T_{rc} should go to zero at $p_B=0.59$. In other words, no phase transition should be present for $0.41<p_B<0.59$. With $J_{AB}>0$ there is a nonzero T_{rc} for all values of p_B. The initial rise in T_{rc} as p_B increases from 0 is greater for larger values of J_{AB}.

The dependence of T_{rc} on J_{AB} for the different p_B values is shown in Fig. 2. The $p_B=0.25$ curve exhibits a slight downward curvature whereas the $p_B=0.75$ curve shows a slight upward curvature. For the $p_B=0.25$ case the B's will exist in many isolated clusters, and for $J_{AB}=0$ their total contribution to the magnetization should be zero. Due to the small value of p_B these clusters will each contain only a few B ions with practically every B having at least one A nearest neighbor. As J_{AB} increases from 0, the B clusters begin to interact with the A background, and the contribution of the B spins to the

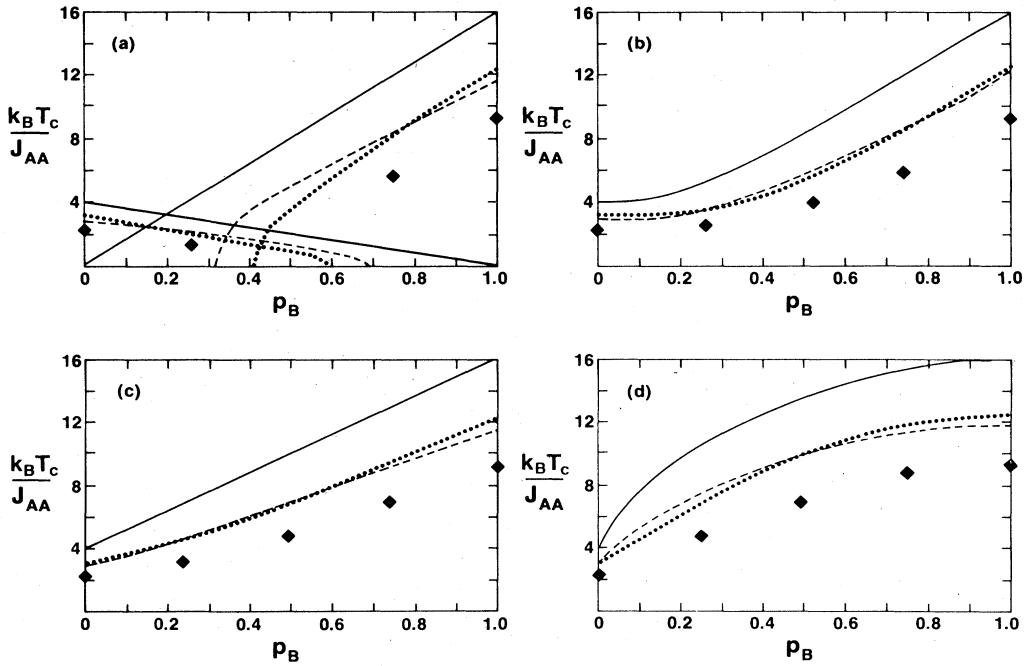

FIG. 3. Comparison of mean-field, ——; Bethe-Peierls, — — —; and HKFK, · · · ·, theoretical results with the Monte Carlo results, ◆, for $k_B T_c/J_{AA}$ as a function of B-ion concentration. Cases shown are (a) $J_{AB}/J_{AA}=0$, (b) $J_{AB}/J_{AA}=1$, (c) $J_{AB}/J_{AA}=2$, and (d) $J_{AB}/J_{AA}=4$.

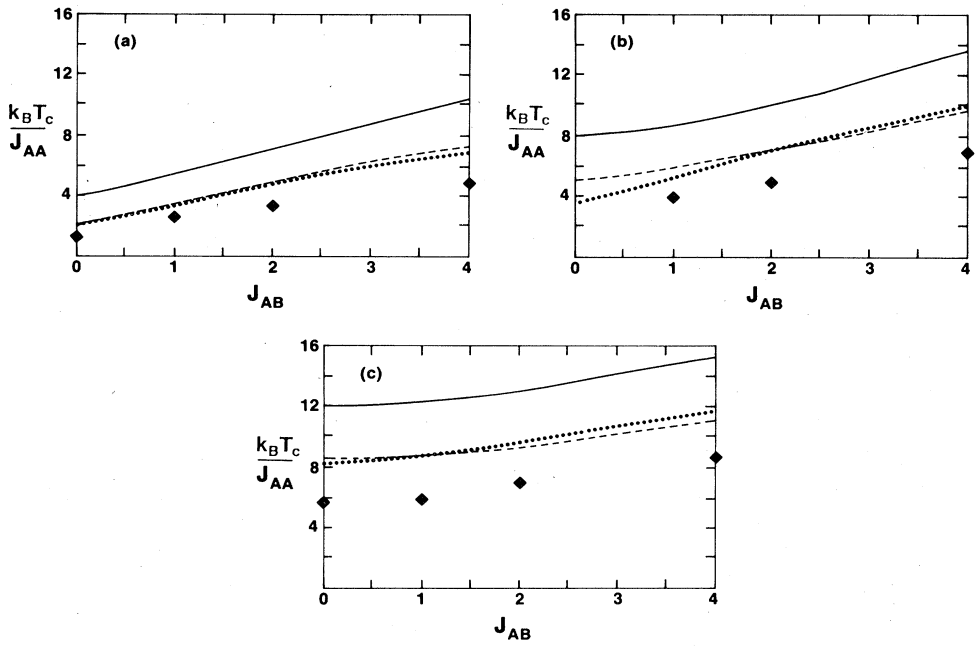

FIG. 4. Comparison of mean-field, ——; Bethe-Peierls, — — —; and HKFK, · · · ·, theoretical results with the Monte Carlo results, ◆, for $k_B T_c/J_{AA}$ as a function of J_{AB}/J_{AA}. Cases shown are (a) $p_B=0.25$, (b) $p_B=0.50$, (c) $p_B=0.75$.

system magnetization is no longer zero. It is during this initial change in J_{AB}, when 25% of the spins suddenly begin interacting with the remaining 75%, that T_{rc} will increase the most, relative to other changes in J_{AB}.

For the case of $p_B=0.75$, Fig. 2 shows the greatest change in T_{rc} to occur when J_{AB} first drops below 4. The analysis of this case is similar to that of $p_B=0.25$. Here, the system consists of isolated A clusters in a B-rich background. When $J_{AB}=J_{BB}$, the A ions are strongly coupled to the B background and many, those with 3 or 4 B

TABLE II. Comparison of ratios of reduced critical temperature (Monte Carlo:theoretical) for mean-field, Bethe-Peierls, and HKFK theories.

p_B			$\frac{(k_B T_c/J_{AA})_{MC}}{(k_B T_c/J_{AA})_{theory}}$		
Nominal	Actual	$\frac{J_{AB}}{J_{AA}}$	Mean field	Bethe-Peierls	HKFK
0.000	0.000		0.572±0.002	0.792±0.003	0.741±0.003
0.250	0.265	0	0.459±0.003	0.659±0.005	0.685±0.005
	0.263	1	0.466±0.002	0.728±0.003	0.741±0.003
	0.239	2	0.475±0.003	0.692±0.004	0.697±0.004
	0.253	4	0.452±0.002	0.654±0.003	0.691±0.003
	0.260	4	0.457±0.002	0.659±0.003	0.695±0.003
0.500	0.520	1	0.441±0.001	0.661±0.002	0.719±0.002
	0.494	2	0.486±0.002	0.698±0.003	0.698±0.003
	0.497	2	0.492±0.001	0.705±0.001	0.705±0.001
	0.494	4	0.509±0.002	0.715±0.003	0.699±0.003
0.750	0.751	0	0.466±0.001	0.667±0.001	0.686±0.001
	0.744	1	0.478±0.002	0.681±0.002	0.684±0.002
	0.751	1	0.488±0.002	0.694±0.003	0.696±0.003
	0.740	2	0.536±0.002	0.753±0.002	0.729±0.002
	0.751	4	0.562±0.001	0.782±0.002	0.737±0.002
1.000	1.000		0.572±0.001	0.792±0.001	0.740±0.001

neighbors, effectively act similar to B ions. As J_{AB} decreases, the A ions decouple from the B background at a temperature lower than the ordering temperature of the B ions. This decoupling of the A's weakens the long-range order in the entire system resulting in a decrease in the system critical temperature.

The Monte Carlo results were compared with those of mean-field theory (MFT),[2,3] the Bethe-Peierls (BP) approximation,[4] and the recent effective-field theory of Honmura, Khater, Fittipaldi, and Kaneyoshi (HKFK).[5] The MFT results for the cases studied in this work appear in Figs. 3 and 4. Although MFT is analytically simple, this approximation omits all details of local interactions and seriously overestimates the value of T_{rc} in all cases. Furthermore, a fundamental difference between MFT and the MC results occurs for the case of $J_{AB}=0$. As mentioned above, there should be no transition when neither p_A nor p_B is below the critical percolation value of 0.59 for the two-dimensional square lattice. Mean-field theory, however, does not take spatial dimensionality into account and predicts the existence of two ordering temperatures for all values of p_B (except for $p_B=0.0$, 0.20, and 1.00).

BP approximation treats the interactions between a spin and its nearest neighbors exactly but considers those neighboring spins to interact with the rest of the lattice via a mean field. The results of the BP are more accurate than those of MFT but are still too high as shown in Figs. 3 and 4. This overestimation of T_{rc} is not at all unexpected considering that the BP result for the pure two-dimensional Ising system is significantly higher than the Onsager (exact) result. As was the case with MFT, the BP is not sensitive to the spatial dimensionality of the lattice and so predicts two transition temperatures for a range of p_B values for the $J_{AB}=0$ case. At about the same level of accuracy as the BP approximation is the HKFK theory. The only significant difference between the two occurs for the case of $J_{AB}=0$ as shown in Fig. 3(a), where the HKFK double-transition region is narrower.

A useful quantitative comparison between the Monte Carlo results and each of the above theories can be made by examining the ratios of predicted T_{rc} (Table II). The most outstanding feature is that the T_{rc} ratios within each section of the table are significantly different. That is, the Monte Carlo results cannot be obtained by simply multiplying all the results of any one theory by a scaling factor. This conclusion remains unchanged even if the error bars are increased to the 1% value estimated above. In terms of the phase diagrams shown in Fig. 3, the differences in these ratios mean that the shapes of the phase boundaries found from the MC method are actually different from those predicted by the theories.

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