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LETTER TO THE EDITOR

Ising ferromagnet with quenched impurities

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Abstract. Using the Monte Carlo technique we have studied a two-dimensional Ising model with quenched non-magnetic impurities. In particular we calculated the temperature dependence of the order parameter, of the zero-field susceptibility and of the specific heat. These results indicate that a second-order phase transition is preserved for $p \geqslant 0{\cdot}9$ where $1-p$ denotes the concentration of randomly distributed non-magnetic sites. Moreover, they yield $\beta \approx 1/8$ and $\gamma \approx 7/4$, indicating that these exponents equal the corresponding ones for the pure Ising model.

An interesting problem in the field of phase transitions is how do quenched non-magnetic impurities influence critical behaviour? Mathematically, the free energy for these systems is obtained by averaging the free energy over impurity configurations (Brout 1959). Very little is known about the behaviour near phase transitions in such systems. Several options are open. The transition could be sharp or smeared (McCoy and Wu 1973). If it is sharp, it could be first or second order. If it is second order, the critical exponents could be those of the pure system or they could be renormalized. Attempts to distinguish these cases in Ising models involve high-temperature expansions (Rushbrooke 1971, Rapaport 1972, and references therein) and the renormalization group approach (Grinstein and Luther 1976, D E Khmelnitzkii 1975, unpublished report). These high-temperature expansions, however, give inconclusive results. The renormalization group approach predicts (Grinstein and Luther 1976, Khmelnitzkii 1975, unpublished report) that there will be a sharp transition with pure system exponents if the specific heat exponent α of the pure system is negative, and a sharp transition with new exponents if α is positive. If $\alpha = 0$, as in the pure $d = 2$ Ising model the renormalization group analysis suggests pure system singularities with some sort of logarithmic corrections. However, Domb (1972) on the basis of diagrammatic analysis of series expansions states that the critical exponents are the same as for the undiluted model. He also gives a formula for the first-order change in the critical point of $\mathrm{d}T_c/\mathrm{d}p$.

In the present letter we present Monte Carlo results for square 55×55 and 110×110 Ising lattices with nearest-neighbour interactions, having quenched and randomly distributed non-magnetic impurities. The systems were subjected to periodic boundary conditions. For a detailed discussion of our Monte Carlo procedure and its reliability we refer to Stoll *et al* (1973). In contrast to that work, however, we introduced non-magnetic and randomly distributed sites with concentrations $1-p$. In particular, we calculated the temperature dependence of the order parameter, of the

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zero-field susceptibility and of the specific heat for $p = 1, 0{\cdot}95, 0{\cdot}9$ and $0{\cdot}8$. Our results indicate that a second-order phase transition is preserved for $p \geqslant 0{\cdot}8$. To illustrate this conclusion more precisely we show in figures 1, 2 and 3 the calculated temperature dependence of the order parameter, of the susceptibility and of the specific heat, respectively. For comparison we include in figure 1 the expression (full line)

$$f(m) = 1 - \frac{\ln(\sqrt{2}+1)}{\ln(1+\{1+[1-(m/p)^8]^{1/2}\}^{1/2}) - \frac{1}{4}\ln[1-(m/p)^8]}. \tag{1}$$

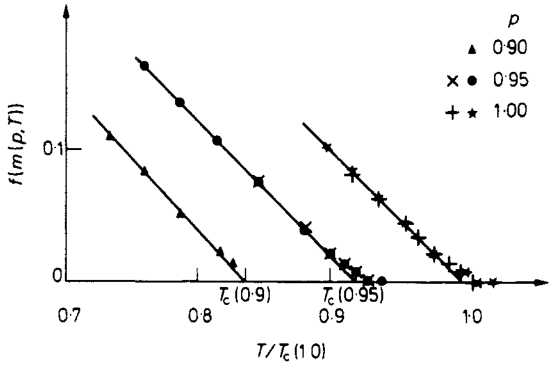

Figure 1. Calculated temperature dependence of the order parameter m for $p = 0{\cdot}9, 0{\cdot}95$ and $p = 1$. $T_c(1)$ denotes the transition temperature of the pure system. $f(m)$ is defined in equation (1). The full line represents the best straight line through the data, excluding the points affected by finite size rounding. ▲, ● and $*$ are results of 110×110 spin systems, whereas $\times$ and $+$ are those of 55×55 spin systems. From the straight lines we estimated $T_c(0{\cdot}95) = 0{\cdot}918\ T_c(1)$ and $T_c(0{\cdot}9) = 0{\cdot}837\ T_c(1)$.

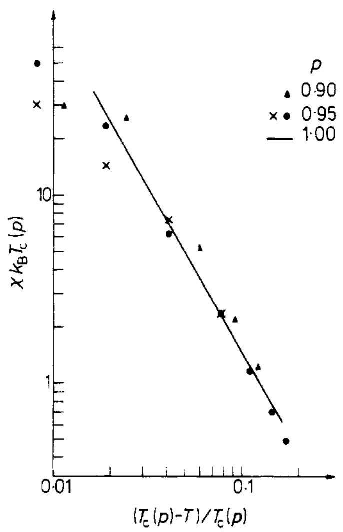

Figure 2. Calculated temperature dependence of the isothermal susceptibility for $p = 0{\cdot}95$ and $p = 0{\cdot}9$. ▲ and ● are susceptibilities of 110×110 spin systems, and $\times$ those of 55×55 spin systems. The full line corresponds to the asymptotic behaviour obtained from series expansions and exact solution of the pure system ($p = 1$) (Fisher 1967).

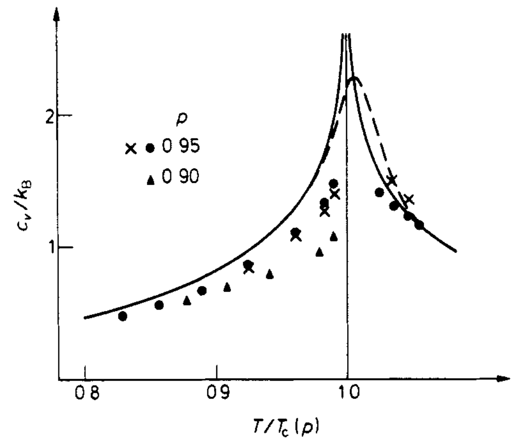

Figure 3. Calculated temperature dependence of the specific heat for $p = 0{\cdot}9$ and $p = 0{\cdot}95$ for 110×110, (▲ and ●) and 55×55 (×) Ising spin systems. The full line corresponds to the exact specific heat of the pure system and the broken one to a pure 64×64 lattice, as obtained by Ferdinand and Fisher (1969).

For $p = 1$, equation (1) reduces to the Onsager formula

$$f(m) = \frac{T_c(p=1) - T}{T_c(p=1)}, \tag{2}$$

for the pure square lattice with nearest-neighbour interaction. From figure 1 it is seen that our data are consistent with

$$f(m) = \frac{T_c(p) - T}{T_c(1)}, \qquad T_c(p) \geqslant T, \tag{3}$$

excluding a narrow region close to $T_c(p)$, which is affected by rounding size effects (Stoll and Schneider 1972). Consequently, our data indicate that $\beta = 1/8$ is preserved for $p \geqslant 0{\cdot}9$. This conclusion is further supported by the calculated asymptotic temperature dependence of the susceptibility shown in figure 2, yielding $\gamma \approx 7/4$. The deviations from the straight line around $(T_c(p) - T)/(T_c(p)) \approx 0{\cdot}01$ are again due to the above mentioned finite size rounding effects. For comparison we included the asymptotic behaviour of the pure system (Fisher 1967).

The temperature dependence of the specific heat is shown in figure 3. For comparison we included the behaviour of the pure infinite and a pure 64×64 system (Ferdinand and Fisher 1969). By approaching $T_c(p)$ from below the difference from the pure-system behaviour is seen to increase. Moreover, these derivations increase with increasing dilution. From the corresponding susceptibility results (figure 2) and the agreement between the specific-heat results for the 55×55 and 110×110 systems, we conclude that these results are not affected by finite size effects. It should be emphasized that our results do not exclude the occurrence of a logarithmic singularity. They reveal, however, that if there is such a singularity, its amplitude will decrease with increasing dilution. Above $T_c(p)$, our results are less conclusive and more data are needed.

Finally we give our result for the first-order change in the critical point

$$\frac{\mathrm{d}w_c}{\mathrm{d}p} = -\alpha w_c, \tag{4}$$

where $w_c = \tanh(J/k_B T_c)$ with $\alpha \approx 1{\cdot}45$. This result can be compared with the prediction of Domb (1972) ($\alpha \approx 1$).

To summarize, our Monte Carlo results obtained for a square Ising model containing quenched and randomly distributed non-magnetic sites of concentration $1-p$, indicate that a second-order phase transition is preserved for $p \geqslant 0{\cdot}9$. The finite size effects turned out to be considerably stronger than in the corresponding pure systems. Nevertheless, our results suggest that the physical picture emerging from the renormalization group approach (Grinstein and Luther 1976, Khmelnitzkii 1975, unpublished report) is correct.

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