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Percolation as the zero-temperature limit of the dilute Ising model

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Abstract. It is shown that, by taking the zero-temperature limit of the annealed dilute bond Ising model, approximate expressions for quantities of interest in the percolation problem can be obtained. These are compared with computer simulations for a square lattice and shown to be reasonable over the entire concentration range whilst giving incorrect critical exponents.

It is well known that at zero temperature the dilute Ising model becomes a percolation problem (see e.g. Essam 1972). This connection has been exploited by taking results for the percolation problem mainly computer simulations and series expansions (see e.g. Shante and Kirkpatrick 1971), and using them to obtain the properties of the dilute Ising model at zero temperature. The most obvious of these is the magnetisation $M(p)$ as a function of the fraction p of occupied bonds, which becomes the probability $P_s(p)$ that a site is part of an infinite cluster. Other correspondences are discussed below.

We note in passing that much more attention (Kasteleyn and Fortuin 1969, Fortuin and Kasteleyn 1972, Harris *et al* 1975) has been paid to the $s \rightarrow 1$ limit of the s -state Potts model. A dimensionless temperature t can be defined by $p = 1 - \exp(-1/t)$, so that as t goes from 0 to ∞ we go from $p = 1$ (all bonds occupied) to $p = 0$ (no bonds occupied) in the percolation problem. An approximation to the percolation problem can be obtained by doing mean field theory on the Potts model and letting $s \rightarrow 1$ (Stephen 1977). The mean field percolation concentration $p_c = 1 - \exp(-1/z) = 0.22$ for the square net ($z = 4$). This is not very close to the exact answer $p_c = 0.5$ (Essam 1972). Mean field theory becomes better as the number of neighbours increases.

Kasteleyn and Fortuin (1969) showed that the analogue of the lattice free energy for the percolation problem is the quantity $\langle \gamma_c(p) \rangle$, the average number of distinct connected clusters per bond for the *bond percolation* model in which each site has the same probability p (or $q = 1 - p$) of being present (or absent). This quantity can be obtained from the *entropy* $S(p, T)$ per bond of the dilute bond Ising model at zero temperature, where each *cluster* behaves like a spin $\frac{1}{2}$ and has an entropy $k_B \ln 2$ associated with it:

$$\langle \gamma_c(p) \rangle = S(p, 0) / k_B \ln 2. \quad (1)$$

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A quantity $C(p)$, which is analogous to a specific heat, can then be obtained (Kirkpatrick 1976):

$$C(p) = (q \, d/dq)^2 \langle \gamma_c(p) \rangle. \tag{2}$$

We also define for the bond percolation problem the fraction $P_s(p)$ of *sites* in the infinite cluster and the fraction $P_b(p)$ of *bonds* in the infinite cluster. It is clear that if the magnetisation per site of the dilute bond Ising model is $M(p, T)$, then

$$P_s(p) = M(p, 0). \tag{3}$$

These expressions can be used to obtain information about the magnetic problem at zero temperature from the percolation problem, which is clearly the simpler of the two. However, Thorpe and Beeman (1976), following earlier work of Rapaport (1972) and Syozi and Miyazima (1966), have obtained an approximation to the dilute bond Ising model, and we shall compare the zero-temperature limit of this annealed bond model (QB) with Monte Carlo results for the percolation problem.

The solution to the dilute quenched bond (QB) Ising model involves an average over the logarithm of the partition function that makes the problem intractable. However, it is possible to construct a grand canonical ensemble in which the bonds are mobile. This leads to the AB model, where, in the thermodynamic limit, the total number of occupied bonds becomes fixed, although correlations are introduced between the positions of the occupied bonds. These correlations are greatest near the critical point and extremely small outside the critical region. The phase diagram is shown in figure 1. Although the

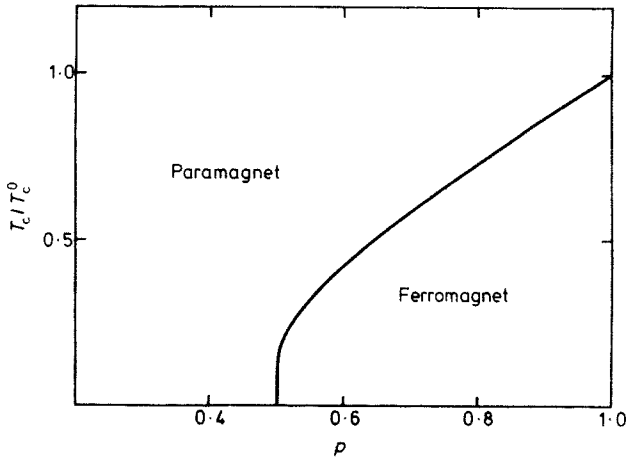


Figure 1. The phase diagram for the dilute annealed bond Ising model (AB) on the square lattice. The phase boundary is given by $\exp(2J/k_B T_c) = (2p + \sqrt{2} - 1)/(2p - 1)$, where T_c^0 is the solution with $p = 1$.

complete QB phase diagram is not known exactly, some portions are. At small $q = 1 - p$ the slope is determined by single missing bonds, and for a square lattice

$$T_c/T_c^0 = 1 - 2q(2 - \sqrt{2})/\ln(1 + \sqrt{2}) \dots \tag{4}$$

The AB model also gives this result. Near the critical concentration $p_c = \frac{1}{2}$, the QB phase boundary has been shown to have the form (Bergstresser 1977)

$$\exp(-2J/k_B T) = A(p - p_c), \tag{5}$$

and by an argument that is probably rigorous Domany (1978) has shown that $A = 2 \ln 2 = 1.387$. The phase boundary of the AB model also has the form of equation (5) with $p_c = \frac{1}{2}$ (this comes about because the square lattice is self-dual (Essam 1972)), but with $A = \sqrt{2} = 1.414$. Thus the phase boundary of the AB model as shown in figure 1 must be very close to the exact (QB) phase boundary. The critical exponents of the AB model are renormalised, so if the subscript 'd' refers to the disordered system and the unsubscripted exponents refer to the pure system with $p = 1$, then

$$\alpha_d = -\alpha/(1-\alpha), \quad \beta_d = \beta/(1-\alpha), \quad \gamma_d = \gamma/(1-\alpha), \quad (6)$$

and exponents that do not involve a temperature derivative like δ are unchanged, so that $\delta_d = \delta$.

The zero-temperature solution of the AB model is expressed in terms of parameters K and $\epsilon(K)$, which are the interaction and nearest-neighbour correlation function $\langle \sigma_1 \sigma_2 \rangle$ of the two-dimensional Ising model (Onsager 1944). The quantity $\epsilon(K)$ can be expressed as an elliptic integral. The concentration p is given by

$$2p = [1 - \exp(-2K)](1 + \epsilon(K)), \quad (7)$$

and the magnetisation $M(p, 0) = P_s(p)$ by (Yang 1952)

$$P_s(p) = [1 - \sinh^{-4}(2K)]^{1/8}. \quad (8)$$

The fraction of bonds in the infinite cluster can also be calculated from $\langle f^{12}(\sigma_1 + \sigma_2) \rangle / 2$, where f^{12} is the indicator function (see Thorpe and Beeman 1976) for occupation of the bond with spins σ_1 and σ_2 at either end. We find that

$$P_b(p) = [2p/(1 + \epsilon(K))]P_s(p). \quad (9)$$

These results are shown in figure 2. It can be seen that the AB results are always below the Monte Carlo results for $P_s(p)$ and $P_b(p)$, although very close for $P_b(p)$. Small

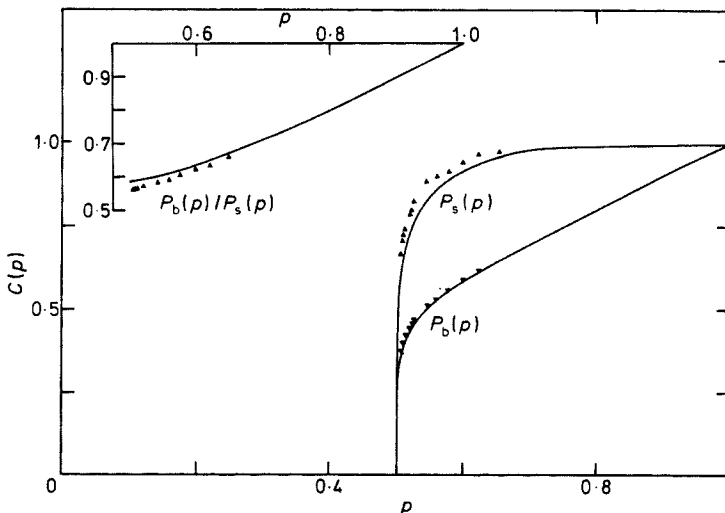


Figure 2. The AB results (full curves) and the Monte Carlo results (triangles) for the percolation probabilities $P_s(p)$ and $P_b(p)$. The Monte Carlo calculations were done on samples ranging in size from 100×100 to 400×400 sites, the larger samples being used near p_c . The inset in the upper left-hand corner shows the ratio $P_b(p)/P_s(p)$.

$q = 1 - p$ expansions for the QB model give

$$P_s(p) = 1 - q^4 \dots, \quad P_b(p) = p(1 - q^6 \dots), \quad (10)$$

whereas the AB expressions can be expanded to give

$$P_s(p) = 1 - 2q^4 \dots, \quad P_b(p) = p(1 - 2q^6 \dots). \quad (10a)$$

Thus, although the leading terms have the correct powers, there are discrepancies of a factor of two owing to the tendency of the missing bonds to *cluster* together in the AB model. Near p_c the AB result is

$$p - p_c = [(\sqrt{2} - 1)/\pi] P_s^8(p) \ln(2/P_s^2(p)), \quad (11)$$

leading to an exponent $\beta = \frac{1}{8}$, whereas the Monte Carlo results are consistent with $0.136 \leq \beta \leq 0.150$. The ratio $P_b(p)/P_s(p)$ goes to a constant value at p_c which the Monte Carlo result gives as 0.562 ± 0.001 , whereas AB gives $1/(1 + 1/\sqrt{2}) = 0.586$. This is consistent with the inequality that can be derived by noting that the total number of bonds in an infinite cluster must exceed the total number of sites, so that

$$P_b(p)/P_s(p) > 2/z, \quad (12)$$

where $z = 4$ is the number of nearest neighbours.

The specific heat can be obtained from (1) and (2). However, there is an *entropy of mixing* S_{mix} per bond,

$$S_{\text{mix}} = k_B[-p \ln p - (1-p) \ln(1-p)], \quad (13)$$

that must be subtracted from the AB result before using equation (1) to find $\langle \gamma_c(p) \rangle$, which is then given by

$$\langle \gamma_c(p) \rangle = [S(K)/k_B + 2pK/(e^{2K} - 1) - p \ln(1 - e^{-2K}) + p \ln p + (1-p) \ln(1-p)]/\ln 2, \quad (14)$$

where $S(K)$ is the entropy per bond of the usual Ising model ($p = 1$) and can be obtained from Domb (1960). At the critical concentration (14) gives a value for the mean number of clusters per bond as 0.056, whereas an exact QB calculation by Temperley and Lieb (1977) gives 0.049. Using equations (2) and (14), the specific heat $C(p)$ is given by

$$C(p) = (1-p) \left[\ln \left(\frac{1-p}{p} \right) + \frac{1}{p} + \ln(e^{2K} - 1) - \frac{2(1-p)}{1 - e^{-2K}} \frac{dK}{dp} \right] / \ln 2, \quad (15)$$

where dK/dp is obtained from equation (7). If the specific heat in the regular Ising model ($p = 1$) is divergent, as it is for the square net, then

$$C(p_c) = (1-p_c) \left[\ln \left(\frac{1-p_c}{p_c} \right) + \frac{1}{p_c} + \ln(e^{2K_c} - 1) \right] / \ln 2, \quad (16)$$

which leads to a value of $\frac{1}{4} + 1/\ln 2 = 1.6927$ compared with a Monte Carlo estimate of 1.5. The AB and Monte Carlo results are compared in figure 3. The main discrepancy is near p_c , where the Monte Carlo results give a cusp with $\alpha = \alpha' = -0.6 \pm 0.1$, whereas AB gives a cusp with $\alpha = \alpha' = 0$ (logarithm). Using a series expansion the result for small q is

$$C(p) = 2zq^2 + \dots, \quad (17)$$

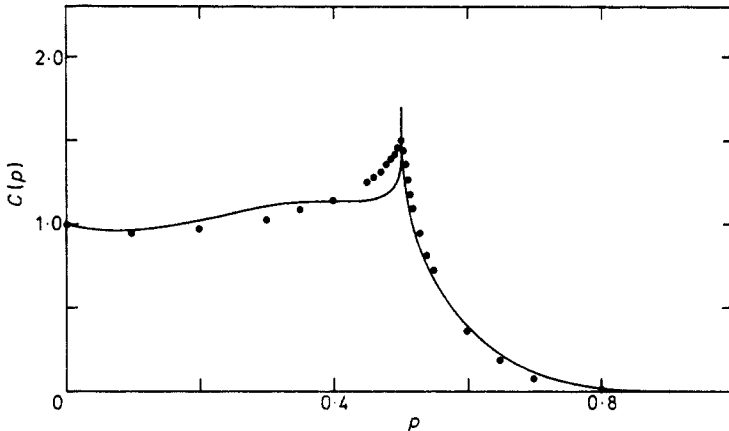


Figure 3. The AB results (full curves) and the Monte Carlo results (circles) for the specific heat $C(p)$ of the square net as defined in equation (2).

whereas AB gives

$$C(p) = 2zq^2/\ln 2 + \dots, \quad (18)$$

with $z = 4$ for the square net.

It is interesting to look at $C(p)$ for the QB Bethe lattice with $z = 3$ (Kirkpatrick 1976) using the generating function of Fisher and Essam (1961). For $p < p_c$

$$C(p) = 1 - p, \quad (19)$$

whereas for $p > p_c$

$$C(p) = q^3(p^3 + 2p^2 + 7p - 4)/p^5. \quad (20)$$

It can be seen from figure 4 that $C(p)$ is continuous at p_c . The AB results can be applied to the Bethe lattice using the expressions for $\epsilon(K)$ and $S(K)$ obtained from the Bethe approximation (Domb 1960). This leads to the same result (19) for $p < p_c$ and to a parametric representation for $p > p_c$,

$$C(p) = \left[\frac{y(1+y^2)}{(1+y)(1+y^3)} \ln \left(\frac{(1+y^2)^2}{1+y^4} \right) + \frac{4y^3(1+y^2)}{(1+y^4)(1+4y^2+y^4)} \right] / \ln 2, \\ p = \frac{1+y^4}{(1+y)(1+y^3)}, \quad (21)$$

where the parameter y is related to the effective field used in the Bethe approximation solution. Above p_c there is considerable discrepancy between the two results. The AB result has a discontinuity $\Delta C = \frac{2}{3}/\ln 2 = 0.9618$, and at small q the two results behave as equations (17) and (18) with $z = 3$. The reason for the disagreement above p_c is that in the ordered phase the Bethe approximation does *not* solve the problem on the Bethe lattice, whereas in the disordered phase below p_c (corresponding to high temperatures) it does (Egarter 1974).

In conclusion we have shown that approximate results can be obtained for the percolation problem by using the results of the annealed bond Ising model (AB). We

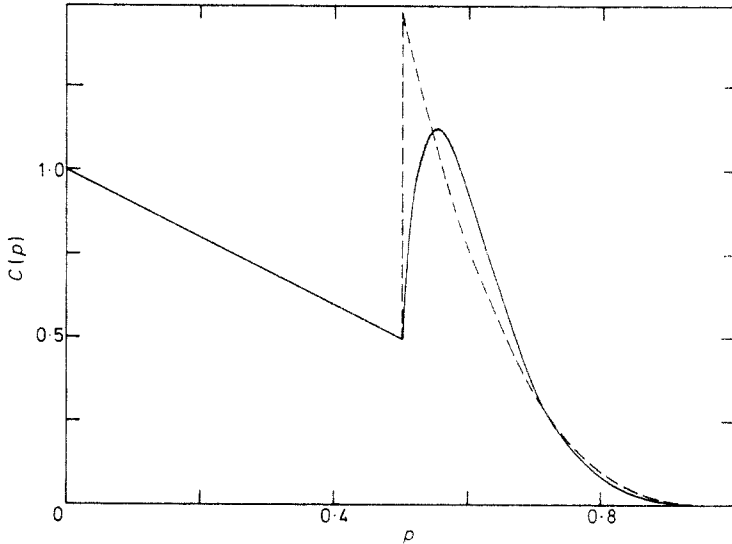


Figure 4. The specific heat $C(p)$ for the Bethe lattice for $z = 3$. The full curve is the exact result, and the broken curve is based on the Bethe approximation using the transformation of Rapaport (1972) and Thorpe and Beeman (1976) for the AB model. Below p_c the two results are identical.

have not been able to obtain expressions for the susceptibility in the percolation problem (see Kirkpatrick 1976, equation (3)) using AB, as the susceptibility of the Ising model ($p = 1$) is not known over the entire temperature range.

Solutions can also be generated in higher dimensions using numerical approximations for $\epsilon(K)$ and $S(K)$. For example, the value of $C(p_c)$ from equation (16) for the simple cubic lattice is 4.06 from Monte Carlo estimates (Kirkpatrick 1976) and 5.10 for AB using estimates from Syozi and Miyazima (1966) ($\epsilon_c(K) = 0.357$ and $\exp(-2K_c) = 0.641$ in equation (7) give $p_c = 0.243$, which is close to the Monte Carlo estimate of $p_c = 0.247$ (Essam 1972)).

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