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LETTER TO THE EDITOR

Renormalisation-group results for bond and site percolation in two and three dimensions

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Abstract. Critical exponents and probabilities are calculated for bond and site percolation on the $d=2$ square lattice and the $d=3$ BCC lattice. The calculation exploits the relationship between the percolation problem and the s -state Potts model in the limit $s \rightarrow 1$. The s -state Potts model is analysed using Kadanoff's variational renormalisation transformation. Results for the critical exponents and critical couplings of the s -state Potts model in the interval $0 < s < 1$ are also presented.

A variety of real-space renormalisation-group techniques has been applied to the percolation problem. The calculations of Harris *et al* (1975) and of Dasgupta (1976) utilise the mapping of the bond-percolation problem onto the s -state Potts model in the limit $s \rightarrow 1$ (Kasteleyn and Fortuin 1969). In the approaches of Young and Stinchcombe (1975), Kirkpatrick (1977), Reynolds *et al* (1977, 1978), Sarychev (1977), and Yuge and Murase (1978) the probabilities rather than an effective spin Hamiltonian are rescaled directly using decimation or site-cell transformations.

Reynolds *et al* (1978) have shown that the site-cell transformation is capable of extremely accurate predictions when combined with Monte Carlo methods so that very large cells can be considered. Of the non-Monte Carlo calculations Dasgupta's work (Dasgupta 1977), in which the s -state Potts model is analysed with Kadanoff's variational transformation (Kadanoff 1975, Kadanoff *et al* 1976), yields the best values for the critical exponents and couplings. Dasgupta considered bond percolation on the $d=2$ square lattice. Recently, Giri *et al* (1977) and Kunz and Wu (1978) have shown that the site-percolation problem can be related to a Potts model with z -spin interactions in the limit $s \rightarrow 1$, where z is the coordination number of the lattice. Using this equivalence and following a procedure similar to Dasgupta's, we have calculated critical exponents and probabilities for bond and site percolation on the $d=2$ square lattice and the $d=3$ BCC lattice.

For details of the Kadanoff variational transformation as applied to the s -state Potts model we refer to Dasgupta (1976, 1977). Our treatments of the bond and site problems differ only in the initial renormalisation transformations we perform. After the initial transformation the Kadanoff transformation as discussed by Dasgupta is applied repeatedly in both cases. One finds the same fixed point and hence the same critical exponents for bond and site percolation.

In the bond-percolation problem the starting Potts Hamiltonian contains nearest-neighbour couplings of the form $K_b \delta_{\sigma_1 \sigma_2}$ where the δ is a Kronecker delta and the spin

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variables σ_i take the values $1, 2, \dots, s$. To avoid problems associated with an extra relevant variable at the fixed point of interest, we initially perform an exact decimation transformation eliminating half the spins in order to enter the invariant 'symmetric subspace' (Burkhardt 1976, Knops 1977) of the Kadanoff transformation. In the square-lattice calculation the decimation leaves a square lattice with expanded lattice constant. In the BCC calculation the decimation eliminates the spins on one of the two simple-cubic sublattices, leaving a simple-cubic lattice.

In the site problem the initial Hamiltonian contains z -spin interactions of the form $K_s \delta_{\sigma_1, \sigma_2, \dots, \sigma_z}^{(z)}$ on the covering lattice of the original lattice of the site problem (Giri *et al* 1977, Kuniz and Wu 1978). The generalised Kronecker delta is defined to be 1 if its z indices are identical and zero otherwise. For site percolation on the square lattice the covering lattice is square, with four-spin interactions in half of the elementary squares, as shown in figure 1. For BCC site percolation the covering lattice is simple cubic, with eight-spin interactions in one-fourth of the elementary cubes. The initial transformation we perform for the site problem is a Kadanoff variational transformation which differs slightly from the usual form of the transformation since the z -spin interactions are not present in every elementary hypercube. Locating the cell spins as shown for $d=2$ in figure 1 and shifting the many-spin interactions into the 'blue hypercubes' produces an effective interaction in the blue hypercube which is a factor 2 times the original interaction instead of the usual factor $z = 2^d$ for interactions initially present in all the elementary hypercubes.

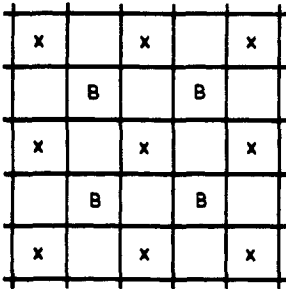


Figure 1. Covering lattice for the $d=2$ square lattice site-percolation calculation. Initially there are four-spin interactions in all the squares with crosses or B's at the centre. The crosses indicate cell spins and the B's label 'blue' squares. Shifting the four-spin interactions into the blue squares produces an effective interaction which is twice the initial interaction.

Following Dasgupta (1976), in computing critical exponents and critical couplings we fixed the variational parameter x in the Kadanoff transformation at the value which maximises $\partial f/\partial s$ at the fixed point, where f is the Gibbs free energy. One maximises $\partial f/\partial s$ rather than f since f becomes independent of s in the limit $s \rightarrow 1$. The x^* determined in this manner is the value to which the function $x^*(s)$, obtained by maximising f at the fixed point with respect to x with s fixed, tends as $s \rightarrow 1$.

The free energy (or $\partial f/\partial s$) can be further maximised by allowing the variational parameter to change each time the renormalisation transformation is applied instead of using the same value in successive applications, as we have done. However, van Leeuwen (1978), van Saarloos *et al* (1978) and den Nijs and Knops (1978) have shown that this procedure leads to an optimum variational parameter which is a singular function of the coupling constants at the fixed point, so that the renormalisation

transformation is also singular at the fixed point. By fixing x at its optimal value at the fixed point, we avoid the non-analyticities and follow the procedure which has yielded the best values for the Ising critical exponents (Kadanoff 1975, Kadanoff *et al* 1976). However, there is some inconsistency in basing the calculation on a variational principle but not using the principle as fully as possible.

Our results for the percolation problem are summarised in table 1 and compared with the values obtained by other methods. Except for p_s^c all the renormalisation-group results given for $d = 2$ were first obtained by Dasgupta (1976). The critical exponents for $d = 2$ calculated with the Kadanoff method agree very impressively with the other estimates. For $d = 3$ the series and Monte Carlo estimates are less precise than for $d = 2$. However, the Kadanoff transformation again seems to yield critical exponents which differ by no more than a few per cent from their exact values. All of the critical probabilities calculated with the Kadanoff method are somewhat too high. The largest discrepancy (about 14%) in the case of p_s^c for $d = 2$ may be a consequence of fixing the variational parameter at its optimum value at the fixed point in each application of the renormalisation transformation. This is a good approximation close to the fixed point but a poorer approximation farther away. In the bond-percolation calculation the exact initial decimation carries the critical Hamiltonian quite close to the fixed point, but in the site-percolation calculation this is not the case. Presumably, introducing an independent variational parameter in each application of the renormalisation transformation would improve the results for the critical probabilities.

Table 1. Calculated values of the critical exponents α, \dots, ν ; of the critical probabilities $p_b^c = 1 - \exp(-K_b^c)$ and $p_s^c = 1 - \exp(-K_s^c)$ for bond and site percolation, respectively; and of the optimum variational parameter x^* . The values in parentheses are exact results or best series or Monte Carlo estimates taken from the summary by Stanley (1977) except where otherwise noted.

	$d = 2$ square lattice	$d = 3$ BCC lattice
α	-0.683 (-0.668 ± 0.004)	-0.678 (-0.58 ± 0.11 ^a)
β	0.139 (0.138 ± 0.007)	0.445 (0.42 ± 0.06, 0.39 ± 0.02)
γ	2.405 (2.38 ± 0.02, 2.43 ± 0.03)	1.79 (1.66 ± 0.07, 1.70 ± 0.11, 1.8 ± 0.005)
δ	18.3 (18.0 ± 0.75)	5.02 (5.0 ± 0.8)
ν	1.34 (1.34 ± 0.02, 1.32 ^{+0.02} _{-0.07})	0.893 (0.83 + 15Δ p_c ± 0.01, 0.825 + 50Δ p_c ± 0.02, 0.86 ± 0.05 ^a)
p_b^c	0.518 ($\frac{1}{2}$)	0.190 (0.178 ^b , 0.1785 ± 0.002 ^d)
p_s^c	0.676 (0.590 ^b , 0.593 ± 0.002 ^c)	0.257 (0.243 ^b , 0.245 ± 0.004 ^d)
x^*	1.25	0.557

- a. Kirkpatrick (1976, 1977)
- b. Shante and Kirkpatrick (1971)
- c. Sykes *et al* (1976a)
- d. Sykes *et al* (1976b)

Dasgupta (1977) and den Nijs and Knops (1978) have studied the x -state Potts model in two dimensions as a function of s using the Kadanoff variational method. The approximation method fails to give a first-order transition for $s > 4$ as predicted by the exact considerations of Baxter (1973). We have found that the Kadanoff method also always predicts a second-order transition for the s -state Potts model in three dimensions. Southern (1978) had previously verified this up to $s = 6$.

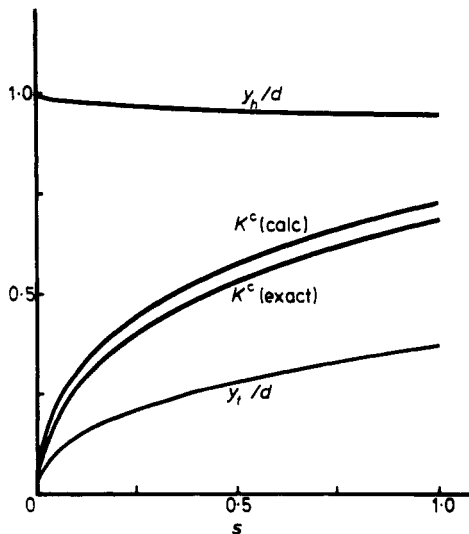


Figure 2. Exact and calculated values of the critical nearest-neighbour coupling K^c , calculated value of the critical indices y_i and y_h for the Potts model on the square lattice in the interval $0 < s < 1$.

For arbitrary s the duality property of the Potts model yields the exact formula (Potts 1952, Kihara *et al* 1954) $K^c = \ln(1 + \sqrt{s})$ for the critical nearest-neighbour coupling on the square lattice. Since $K^c \rightarrow 0$ as $s \rightarrow 0$, one might hope to obtain results for the percolation problem with a weak-coupling expansion about $s = 0$. Kunz and van Leeuwen (Kunz 1977) have examined the predictions of the Migdal recursion formula (Migdal 1976, Kadanoff 1976) for small s . In figure 2 we show results of the Kadanoff variational method in the interval $0 < s < 1$. The calculated K^c , which is systematically larger than the exact value, appears proportional to \sqrt{s} as $s \rightarrow 0$ on a logarithmic plot. The critical indices y_i and y_h also approaches the values 0 and 2 for $s = 0$, respectively, with leading corrections proportional to \sqrt{s} , just as predicted by the Migdal recursion relation. For $d = 3$ the Migdal formula predicts leading corrections which are linear in s . Because of numerical difficulties perhaps associated with the large number of coupling constants in the Kadanoff recursion relation, we were unable to track the fixed point for $d = 3$ to small enough values of s to see the asymptotic form of the leading corrections.

We have seen that the Kadanoff variational method, which yields critical exponents and critical couplings with surprising accuracy for a variety of models, is also quite successful in predicting results for the percolation problem in two and three dimensions. However, the approach is not without disturbing features. As with other real-space renormalisation-group methods the approximations involved are uncontrolled, and it is not clear to what extent the impressive predictions of critical exponents are fortuitous. We have already referred to the difficulties encountered in trying to improve the method by optimising with a different variational parameter at each step. Although the approach of Reynolds *et al* (1978) to the percolation problem requires Monte Carlo numerical techniques, it has the advantages of permitting systematic improvement of the approximation and error estimates.

Note added in proof. Exact dual and decimation transformations may be used to replace the starting Hamiltonian in the square-lattice site-percolation problem, which contains

four-spin interactions in half of the squares, by an equivalent Hamiltonian with four-spin couplings in every square (to be published). The coupling strengths K_s and \hat{K}_s of the original and equivalent four-spin interactions satisfy $\exp(-K_s) = 1 - \exp(-\hat{K}_s)$. Prefacing Kadanoff's recursion relation with these exact transformations instead of the initial bond-shifting approximation described above leads to a considerably improved result for the critical probability for site percolation. One obtains $p_s^c = 0.569$.

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