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Critical behaviour of *AB* percolation in two dimensions

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Abstract. Monto Carlo simulation of the *AB* percolation model on large triangular lattices gives indications that this problem has the same set of critical exponents as ordinary percolation although a critical amplitude ratio, which is thought to be universal, appears to be significantly different from accepted values for two-dimensional percolation. In addition, finite-size scaling functions for both the percolation probability and susceptibility seem to be significantly different from those for ordinary percolation in two dimensions. We also show that this problem is closely connected to that of the percolation hull and in fact is dual to the complement of the hull problem.

1. Introduction

AB percolation is a connectivity problem in which connection exists only between neighbouring *unlike* species *A* and *B* and *not* between like species such as *A* and *A* or *B* and *B*. This problem is usually discussed as an example falling in a group of percolation problems called polychromatic percolation (for which there are several excellent reviews; see, e.g., Halley (1983) and references therein). In particular, in this paper we consider each site of a triangular lattice to be occupied at random (and independently) by an *A* particle with probability p and by a *B* particle otherwise and consider connectivity between nearest-neighbour *AB* pairs only. It is clearly a relevant model if one wants to study a gelation problem where crosslinking occurs only between two unlike monomers constituting the gel. Other applications are also discussed in the already formidable literature on polychromatic percolation.

In view of the simplicity of the problem and of the potential usefulness, it is rather surprising that there is apparently no agreement on the nature of the critical point of *AB* percolation. On the one hand, Mai and Halley (1980) conclude, based on Monte Carlo simulations on the triangular lattice, that it is in a different universality class from the usual two-dimensional percolation while, on the other hand, Sevšek *et al* (1983) conclude from phenomenological renormalisation that it is in the same universality class. To be sure, there are points all seem to agree on: (i) in three dimensions they are probably in the same universality class and (ii) for lattices consisting of two sublattices with ordinary site percolation threshold greater than $\frac{1}{2}$ there is no transition. Still, on the triangular lattice, which appears to be the only regular two-dimensional lattice supporting infinite *AB* connectivity, there is a fundamental disagreement.

Since Mai and Halley (1980) calculated the critical exponents β (for the percolation probability) and γ (for the susceptibility) (for the definition of these exponents, see the review by Stauffer (1979)) and since Sevšek *et al* (1983) calculated ν (for the connectedness length), one possibility is that the 'thermal' eigenvalue is the same for

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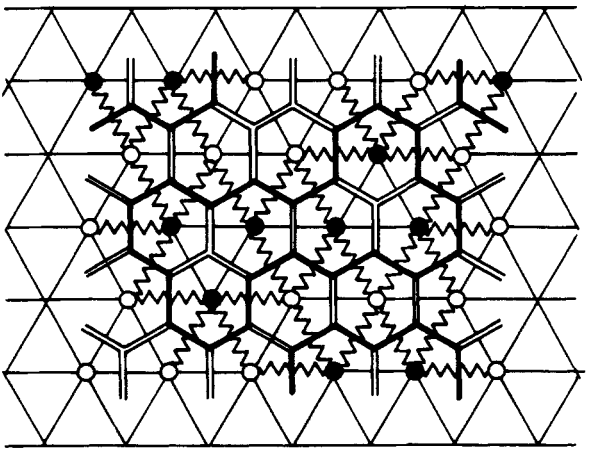

Figure 1. Duality transformation is illustrated from a bond configuration of AB percolation on a triangular lattice (shown in zigzag lines) to one on a honeycomb lattice (shown in double lines). The full circles represent A (B) particles and open circles represent $B(A)$ particles. This figure also shows the percolation hull in bold lines on the dual honeycomb lattice (which is just the complement of the double lines). Notice that the hull is a collection of non-intersecting polygons and that within the particular hull cluster shown here there are three disconnected clusters made of the double lines.

both problems while the 'magnetic' one is different. If this were true, it would be interesting since this is the opposite of usual 'extended' universality (Suzuki 1974). (However, we also note that it would be similar to the relationship between the percolation hull problem and the percolation problem (Ziff 1986).) This is one reason why it is interesting to perform a much larger scale Monte Carlo simulation on this problem.

Yet another reason for which such an undertaking is of interest is that this problem is *dual* to the one whose cluster configurations (with proper weights) are obtained as the complement of the polymerisation problem with only rings on the honeycomb lattice as discussed in the following section. The latter problem is otherwise known as the percolation hull problem for site percolation on the triangular lattice (see figure 1). It is easy to see this because each configuration with only rings on the honeycomb lattice is the result of connecting together the bonds which cross the *perimeter* bonds for site percolation clusters on the dual triangular lattice. The hull problem has been solved recently by a mapping to a Coulomb gas (Saleur and Duplantier 1987) and it is now believed that its 'thermal' eigenvalue is the same as for percolation while its 'magnetic' eigenvalue is different, i.e. the exponents ν and α are the same as for percolation while β, γ, etc, are different. So the question is: is AB percolation (which is dual to the complement of the hull) like ordinary percolation or like the hull, or possibly like neither?

2. Duality transformation for AB percolation

AB percolation is normally stated as a *random* site percolation problem. However, since the essential connectivity is defined through *bonds* between A and B particles, it is easier to think of it as a bond percolation problem. This, however, introduces

correlations between bonds and the problem is no longer a random one but a *correlated* one. This situation is illustrated in figure 1 where, e.g., not all three bonds on a triangular unit cell can be present. One is reminded by this of a similar situation which occurred in a model called 'four-coordinated site percolation' introduced by Stanley (1979) in order to model low-density patches in liquid water; in that case, the original problem is a random-bond percolation model but one instead considers it as a correlated-site percolation problem.

The constraint is simply that if one goes around any closed loop on the lattice then one must get back to the same kind of site (in fact that same site), or put another way, that there are even numbers of bonds on any closed loop. For any two-dimensional lattice with no overlapping bonds, this can be further simplified to the following constraint.

(A) On any unit cell, an even number of bonds are occupied.

A unit cell is the smallest repeating segment of the lattice and is triangular on a triangular lattice and square on a square lattice and so on. Thus in our problem on the triangular lattice, there can be only two bonds or none on the unit cell. All bond graphs satisfying this constraint are allowed (in fact each occurs exactly twice because of the AB symmetry) and no other graphs are allowed.

In addition, if p is the probability that a given site is A, then the probability that any given bond is occupied is $2p\ (1-p)$ when no knowledge of any other bond is presumed. Thus the overall concentration q of the bonds in the correlated-bond percolation picture is simply

$$q = 2p(1-p). \tag{1}$$

The problem is now reduced to a constrained bond-percolation problem with constraint (A) and overall bond concentration (1). Since the transformation (1) is analytic in p, all critical exponents given in terms of p are unchanged when given in terms of q except if $p_c = \frac{1}{2}$ where q is a maximum.

To this problem we apply the well known duality transformation (cf Sykes and Essam 1964). As shown in figure 1, each triangular cell is transformed into a vertex with three bonds on a honeycomb lattice, and each of these bonds is occupied if and only if the corresponding bond on the triangular lattice (which crosses it) is *empty*. (It is important to realise that the latter requirement is not symmetric with the one which requires the crossing bonds to be *occupied*!) In this process, the concentration of bonds becomes $1-q$, and the constraint (A) is now replaced by the following new constraint.

(B) Each vertex of the dual lattice is attached to an odd (even) number of occupied bonds if the number of edges of the original unit cell is odd (even).

The duality theorem as extended to the present case states that

$$G(q;\ T(\mathrm{A})) = \phi(q) + G(1-q;\ H(\mathrm{B})) \tag{2}$$

where G is the mean total number of clusters per site and $T(\mathrm{A})$ refers to the problem on the triangular lattice with the constraint (A) while $H(\mathrm{B})$ refers to the dual problem on the honeycomb lattice with the constraint (B). The quantity $\phi(q)$ is a certain polynomial in q having to do with the probabilities of occurrence of certain *faces* in the Kagomé matching lattice which is the covering lattice of the triangular bond lattice (Sykes and Essam 1964). Assuming that there is one singularity in G, duality then has consequences in the estimation of p_c as discussed below and also in the fact that at least the 'thermal' eigenvalue (corresponding to exponents ν and α, etc; see Stauffer (1979)) must be the same for the two problems $T(\mathrm{A})$ and $H(\mathrm{B})$.

The percolation threshold for AB percolation on the triangular lattice was estimated by Mai and Halley (1980) to be $p = 0.2145 \pm 0.0005$ (with another positioned symmetrically about $\frac{1}{2}$) while Sevšek *et al* (1983) estimated it to be about 0.21. We have an independent estimate of p_c from our simulations which is comparable with these as discussed below; however, we can also put this number in an interesting perspective by considering the dual H(B) problem.

First, note that the relationship between the threshold q_c of the original T(A) problem and that q_c^* of the dual H(B) problem follows from the relation given by Sykes and Essam (1964) first formulated for the random percolation problem:

$$q_c + q_c^* = 1. \tag{3}$$

Now the percolation threshold for the *random*-bond problem on the honeycomb lattice is known to be exactly $1 - 2\sin(\pi/18)$ or about 0.6527. If we imagine a typical *random* configuration on the honeycomb lattice at this p_c and try to modify it so that constraint (B) is satisfied, while keeping the same overall bond concentration, we must dismantle some of the bonds attached to two-coordinated sites so that all sites are turned into either one- or three-coordinated ones. This process in general involves trade-offs in connectivity so we do not expect the overall connectivity to change very much; still, since an incipient infinite cluster has many singly connected bonds, one would expect the dismantling of the two-coordinated sites to destroy the incipient infinite connectivity. If this argument is correct, then we will have

$$q_c^* > 1 - 2\sin(\pi/18). \tag{4}$$

This will then yield p_c for the original problem of $p_c \leqslant 0.225$ (with another one symmetrically positioned about $\frac{1}{2}$) which is certainly consistent with the numerical estimates. Incidentally, the closeness of the value obtained from the random percolation problem on the honeycomb lattice with the actually observed p_c lends some support to the idea that the type of transition involved is also close to that of the usual percolation problem.

To cast the problem in another light, let us introduce a new problem on the dual lattice which is defined by the graphs obtained by complementing those satisfying (B) or the following new constraint.

(C) Each vertex of the dual lattice is attached to an even number of occupied bonds.

We note that if the number of edges of the original unit cell is even (e.g. a square lattice) then the constraints (B) and (C) are identical. In the case of a triangular lattice, this new constraint yields a new problem on the honeycomb lattice with each vertex attached to either no occupied bond or exactly two occupied bonds. This translates to the requirement that only connected components allowed on the honeycomb lattice are indefinitely long self-avoiding walks (SAW) or else self-avoiding polygons of any size with the bond concentration q. This is of course just the description of the percolation hull given earlier.

In the case of the square lattice SQ (A), the similarly transformed dual problem SQ (B) is a bond percolation problem, with the bond concentration equal to $1 - q$, again on a square lattice but with a constraint that all vertices are attached to either no, two or four occupied bonds. This allows self-avoiding polygons and four-coordinated crosslinks (as well as indefinitely long SAW). Although this problem is known to have *no* percolation transition (cf Halley 1983) it is interesting to note that this is somewhat similar to so-called restricted-valence percolation problems (Gaunt *et al* 1983). The complement SQ (C) of the dual problem SQ (B) is, interestingly, formally the same

problem as SQ (B) itself. This would appear to mean that the percolation hull for the square-lattice site percolation is dual to the *AB* percolation on the same lattice; however, the bond concentration $1-q$ for SQ (B) is not less than $\frac{1}{2}$ while that q for SQ (C) is always $\frac{1}{2}$ or less and thus they describe the same problem in different regions of the bond concentration. One might surmise then that *AB* percolation on the square lattice has a *transition* if p is analytically continued to complex values and, there, the 'thermal' eigenvalue is the same as that of the hull and thus as that of the ordinary percolation.

3. Monte Carlo results

Previous Monte Carlo calculations by Mai and Halley (1980) used lattices of relatively small size (up to 280×280) and their statistics were not very good by today's standards of similar calculations done for random percolation (see, e.g., Margolina *et al* 1984). They gave surprising values for the critical exponents $\gamma=1.564\pm0.182$ and $\beta=0.121\pm0.004$, quite different from the ordinary percolation values: $\gamma=\frac{43}{18}=2.388\ldots$ and $\beta=\frac{5}{36}=0.1388\ldots$ which are believed to be exact (den Nijs 1979, Nienhuis *et al* 1980, Pearson 1980, Nienhuis 1982). We improve the statistics by using lattices of four successive sizes, namely, 1000×1000, 2500×2500, 5000×5000, and $10\,000\times10\,000$ where for each lattice size we simulate percolation clusters with free boundaries at seventeen different values of p from 0.180 to 0.245. The total number of samples used range from 100 for $10\,000\times10\,000$ to 380 for 2500×2500. These improvements are made possible by applying the now well known technique of Hoshen and Kopelman (1976) to this problem; since *AB* percolation involves only two kinds of sites, the modifications required are relatively minor.

As random percolation, for the purpose of computing the percolation probability, the largest cluster stands for the infinite or percolating cluster. The exponent γ is estimated from the divergence of susceptibility which is just the second moment of the cluster-size distribution. Standard techniques of estimating the exponents from the slopes of double logarithmic plots are used in this analysis. A trial estimate of the effective value of p_c is made first; then linear regression is done on the susceptibility against $|p-p_c|/p_c$ on the logarithmic scale. The effective p_c is adjusted to make the resulting estimates of γ (below p_c) and γ' (above p_c) equal. In practice we must decide which region of p to use for the fitting process; we have chosen six values of p (from 0.180 to 0.205) below p_c and five values (from 0.225 to 0.235) above p_c because this region presented good fits consistently for all of the lattice sizes involved. We give in figure 2 such a double logarithmic plot of the susceptibility from the $10\,000\times10\,000$ lattice where the effective p_c ($L=10\,000$) was estimated to be about 0.215 47; this number is only accurate within the particular procedure and would change if, e.g., the fitting region were changed.

The above procedure then yields an effective p_c (L) for each latice size L. To estimate the true p_c for the limit of infinite lattice size, we must extrapolate p_c (L) linearly against $L^{-1/\nu}$ for $L\to\infty$ according to the theory of finite-size scaling (Fisher 1972). Since Sevšek *et al* (1983) explicitly computed ν to be the same as the percolation value of $\frac{4}{3}$, we use this value first to perform the extrapolation. Later we see that this is consistent with our data because the least-squares fit with this value gives reasonable correlation and also because the finite-size scaling is seen to be well satisfied using this estimated p_c and $\nu=\frac{4}{3}$. This procedure of linear least-squares fit yields the estimate

$$p_c=0.215\,24\pm0.000\,34. \tag{5}$$

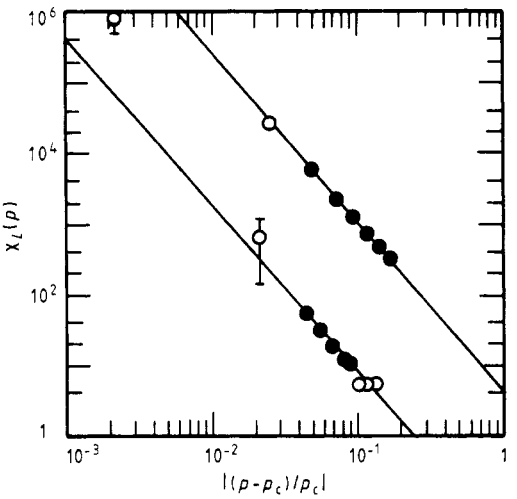

Figure 2. Double logarithmic plot of the susceptibility $\chi = \Sigma' s^2 n_s$ where n_s is the number of clusters per site and the sum runs over all clusters except the largest one. The data are taken from the total of 100 Monte Carlo runs of a $10\,000 \times 10\,000$ triangular lattice distributed over seventeen values of p (from 0.180 to 0.245). The straight lines drawn are the least-squares fits to the points shown as full circles only but they are also reasonable fits to all the points except the two that are shown with large error bars. These correspond to $p = 0.125$ and $p = 0.220$, namely the two values of p closest to the estimated p_c. The standard errors of all other points are smaller than the symbols used and in most cases far smaller. The two lines shown give $\gamma = 2.38$ and the amplitude ratio $R = 145$.

The quoted error range is from the least-squares fit and does not reflect any systematic error in the values p_c (L) for each L if there were any.

The estimates of the exponent γ and the amplitude ratio R for the susceptibility above and below p_c are made for each L in the above procedure. The final estimates of γ and R with associated errors are made somewhat crudely by simply taking the average of the estimates from the four lattice sizes with no consideration of relative weights; however, the final estimates are quite consistent with the values obtained from the largest lattice ($L = 10\,000$) alone:

$$\gamma = 2.39 \pm 0.09 \tag{6}$$

and

$$R \equiv C_+ / C_- = 139 \pm 24. \tag{7}$$

In both cases, the quoted errors are only those due to the standard error of the four estimates from the four sizes; there may be substantial additional systematic errors not accounted for.

While the estimate for γ is very close to that of the ordinary percolation discussed before, the amplitude ratio R for susceptibility is significantly different from the ordinary percolation value of about 200 (cf Nakanishi and Stanley 1980). This situation is quite similar to two other cases known to us, namely continuum percolation and kinetic gelation. In two-dimensional continuum percolation, Gawlinski and Stanley (1981) asserted on the basis of Monte Carlo simulations that all the exponents are the same as ordinary lattice percolation but the corresponding amplitude ratio (according to certain definitions of the *size* of a cluster) is about 50 instead of 200. In kinetic

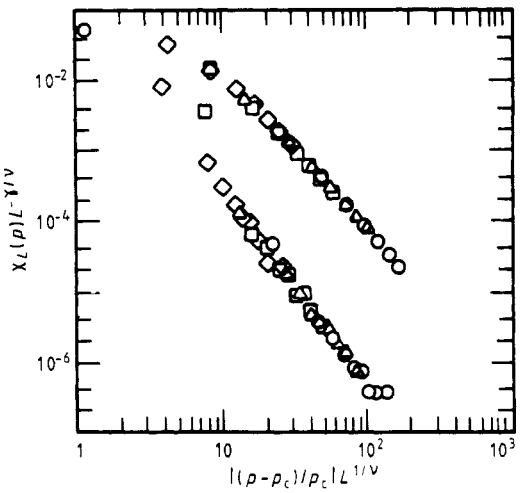

Figure 3. The finite-size scaling function $\chi_L L^{-\gamma/\nu}$ is shown as a function of $|(p-p_c)/p_c|L^{1/\nu}$. L is the linear size of the lattice from 1000 (◇), 2500 (□), 5000 (△) and 10 000 (○) and χ_L is the susceptibility. The value of 0.215 24 used for p_c is the estimate obtained in this work and those for the critical exponents are the random percolation ones (see text).

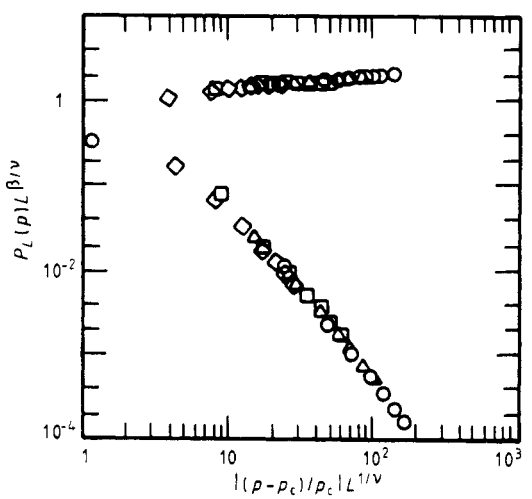

Figure 4. The finite-size scaling function $P_L L^{\beta/\nu}$ is shown as a function of $|(p-p_c)/p_c|L^{1/\nu}$. L is the linear size of the lattice from 1000 (◇), 2500 (□), 5000 (△) and 10 000 (○) and P_L is the percolation probability (the fraction of the largest cluster over all lattice sites). The value of 0.215 24 used for p_c is the estimate obtained in this work and those for the critical exponents are the random percolation ones (see text). We see that the general shape of this function is quite similar to the corresponding function given by Heermann and Stauffer (1980) for the square bond percolation but it cannot be reduced to the same function quantitatively by simple scaling using metrical factors alone.

gelation in three dimensions, the exponents are again estimated to be the same as for three-dimensional percolation while the amplitude ratio R is apparently much smaller (Herrmann *et al* 1982).

The estimate of β is not as reliable as for γ since we use the percolation probability $P(p)$ only on one side of p_c to fit for this exponent. The effective $p_c(L)$ used for the estimation of γ is not necessarily the best one to use for this function as such effective thresholds generally depend upon the function we wish to use them for. If we ignore this problem and use the same $p_c(L)$ and the same five values of $p > p_c$ as used for γ, and if we then take a simple average of the resulting estimates of β, then we obtain $\beta = 0.127 \pm 0.002$. However, the double logarithmic plots of $P(p)$ against $p - p_c(L)$ have systematic curvatures even in the region of fitting, and if we try to locate another effective $p_c(L)$ by seeking the best linearity, then we obtain estimates of β wildly varying from 0.10 to 0.16 depending on L. Thus we think it prudent to quote a loose estimate:

$$\beta = 0.13 \pm 0.03 \tag{8}$$

which is consistent with the ordinary percolation value of about 0.14.

In figures 3 and 4 we give finite-size scaling functions for the percolation probability and susceptibility respectively, using the ordinary percolation exponents (the exact values quoted before for γ, β and ν) as well as the present estimate of $p_c = 0.215\,24$). The degree of data collapsing is excellent for both cases, reinforcing our suggestion that this problem has the same set of exponents as percolation. Also, the general functional dependence of these scaling functions are quite similar to the ordinary percolation counterparts although they do not seem to be quantitatively identical (or related by simple metrical factors) as is obvious from the difference in the amplitude ratio R.

4. Summary

Extensive Monte Carlo simulations suggest strongly that AB percolation has the same set of critical exponents as ordinary percolation supporting the conclusions of Ševšek *et al* (1983) but contradicting the Monte Carlo study of Mai and Halley (1980) which is similar to ours but performed on a much smaller scale. There may, however, be subtle differences between these two problems as the difference in an amplitude ratio suggests. There is an interesting connection between this problem and that of the percolation hull; AB percolation is dual to the complement of the hull. Curiously, for the square lattice, this latter connection reduces to the fact that both the dual of AB percolation and the hull problem derive from the identical rules on the same lattice, however, in different regions of the bond concentration. The former has no transition while the latter has a transition whose 'thermal' eigenvalue is the same as for percolation and whose 'magnetic' one is different. This may also suggest, by analytic continuation of p to a complex region, that the 'thermal' eigenvalue of AB percolation must also be the same as that of ordinary percolation.

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Note added in proof. Recently Meir (1987) has developed a new series analysis technique. Using this method, he has confirmed the Monte Carlo estimate of C_+/C_- for ordinary two-dimensional percolation. Thus it raises the hope that Monte Carlo estimates of such ratios may be quite accurate.

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